Electronic Structure and Absorption Spectra of Biferrocenyl and Bisfulvalenide Diiron Radical Cations: Detection and Assignment of New Low-Energy Transitions

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Supporting Information

1. *Elemental analysis data (cf. Experimental part) :*

Fc_2I_3 : calc.: C: 32.00 %, H: 2.42 %, I: 50.71 %, found: C: 31.88 %, H: 2.36 %, I: 49.63 %;
$(FcEt)_2I_3$: calc.: C: 35.73 %, H: 3.25 %, I: 47.18 %; found: C: 35.58 %, H: 3.34 %, I: 46.83 %;
$Fc{=}FcI_3$: calc.: C: 32.08 %, H: 2.15 %, I: 50.85 %; found: C: 32.04 %, H: 2.19 %, I: 50.93 %

2. *Complete reference for the Gaussian program system (Ref. 35 in the paper):*

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03 Rev. C01, Gaussian, Inc., Wallingford CT, 2004.

3. *Complete reference for the ADF program system (Ref. 39 in the paper)*

E. J. Baerends. J. Autschbach, A. Bérces, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, L. Fan, T. H. Fischer, C. Fonseca Guerra, S. J. A. van Gisbergen, J. A. Groeneveld, O. V. Gritsenko, M. Gruening, F. E. Harris, P. van den Hoek, H. Jacobsen, G. van Kessel, F. Kootstra, E. van Lenthe, D. A. McCormack, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. G. Snijders, M. Sola, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, O. Visser, E. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo and T. Ziegler, ADF2004.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http:// www.scm.com.

4. Figures

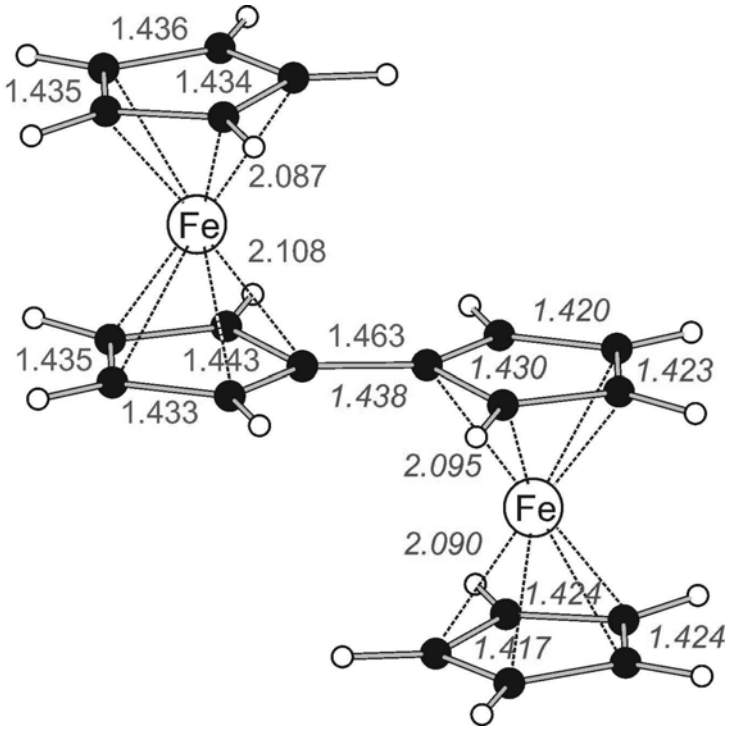

Figure S1: Structures of **Fc_2** and its radical cation, calculated with the ADF program by the BP86/ TZP(ZORA) method, with interatomic distances indicated in normal font for the neutral dimer and in italic for the radical cation.

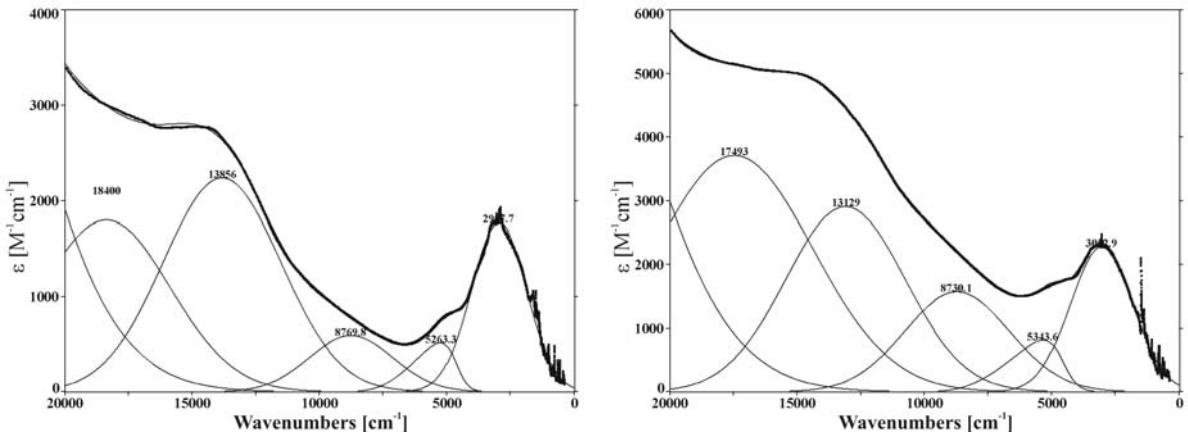

Figure S2 : Peak-fit analysis of the low-energy bands of **Fc_2I_3** (left) and **$(EtFc)_2I_3$** (right) in KBr at 300 K.

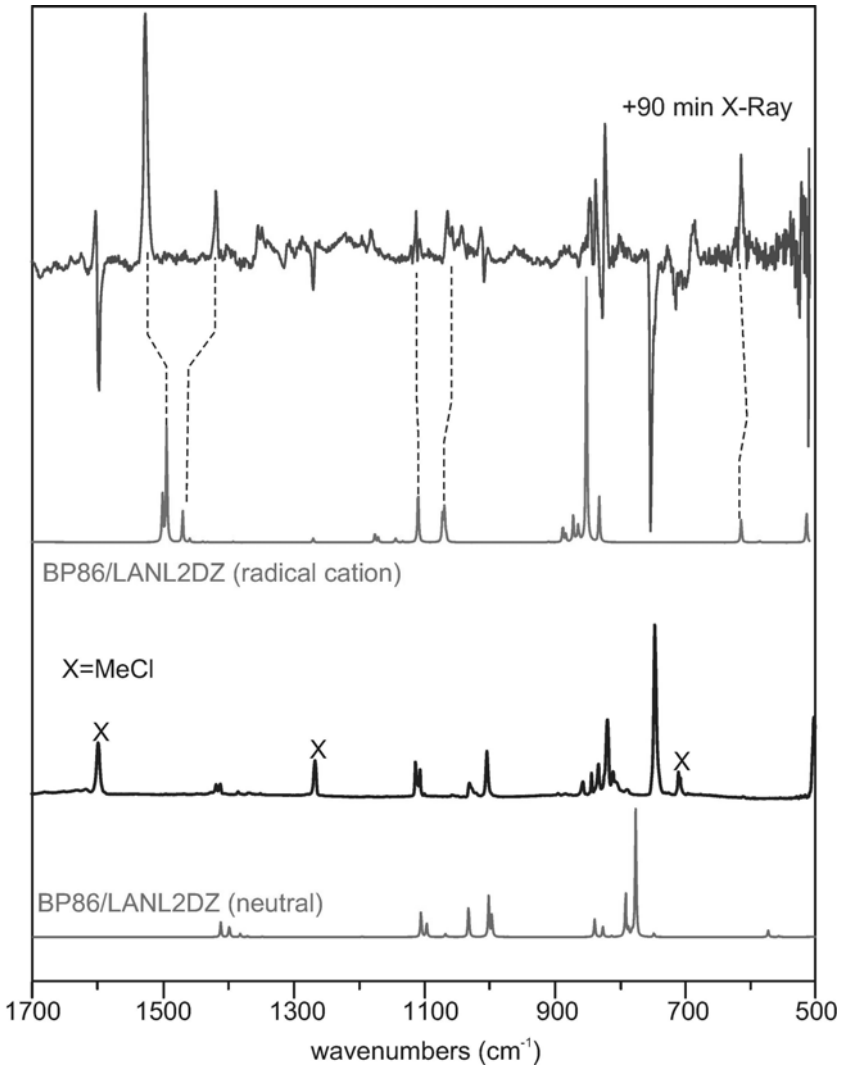

Figure S3: Lower half: IR spectrum of $\mathbf{Fc_2}$ in an Ar matrix (upper trace) and calculated by DFT (bottom). Top: Changes in the IR spectrum of $\mathbf{Fc_2}$ on ionization by X-irradiation in Ar, Center: calculated IR spectrum of $\mathbf{Fc_2}^{\bullet+}$.

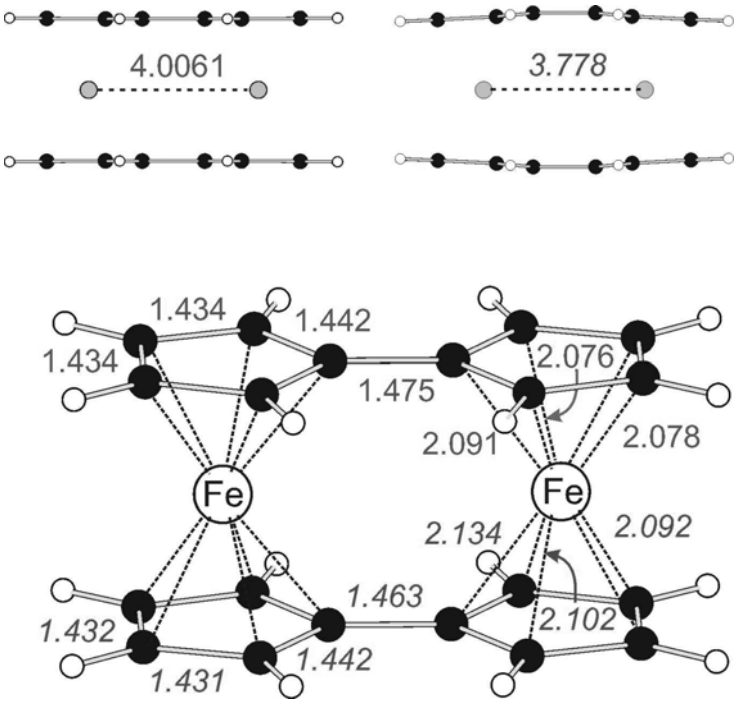

Figure S4: Structures of **Fc=Fc** and its radical cation, calculated with the ADF program by the BP86/ TZP(ZORA) method, with interatomic distances indicated in normal font for the neutral dimer and in italic for the radical cation.

5. Geometries and TD-DFT results

General remarks:

The calculations with ADF were done with the following kind of input:

```
Basis
C /apps/adf2005.01/atomicdata/ZORA/TZP/C.1s
H /apps/adf2005.01/atomicdata/ZORA/TZP/H
Fe /apps/adf2005.01/atomicdata/ZORA/TZP/Fe.3p
end

XC
GGA BP86
end
```

The calculations with Gaussian 03 were run with
the keyword BP86/LANL2DZ

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1. Bisferrocene (Fc2)

a. calculated by ADF

1.XX	-4.741423	0.497199	0.000000
2.C	-3.244399	1.351145	0.000000
3.C	-3.720255	0.654739	-1.160255
4.C	-3.720255	0.654739	1.160255
5.H	-2.611379	2.234841	0.000000
6.C	-4.495706	-0.469861	-0.717442
7.H	-3.523478	0.927746	-2.193927
8.C	-4.495706	-0.469861	0.717442
9.H	-3.523478	0.927746	2.193927
10.H	-4.987075	-1.199494	-1.356249
11.H	-4.987075	-1.199494	1.356249
12.Fe	-2.546147	-0.615830	0.000000
13.XX	-1.039653	-1.729750	0.000000
14.C	-0.438639	-0.585217	0.000000
15.C	-0.955361	-1.273534	1.158657
16.C	-0.955361	-1.273534	-1.158657
17.C	-1.745043	-2.385540	0.717417
18.H	-0.772255	-0.998704	2.193905
19.C	-1.745043	-2.385540	-0.717417
20.H	-0.772255	-0.998704	-2.193905
21.H	-2.265214	-3.092977	1.357899
22.H	-2.265214	-3.092977	-1.357899
23.C	0.438639	0.585217	0.000000
24.XX	1.039653	1.729750	0.000000
25.C	0.955361	1.273534	1.158657
26.C	0.955361	1.273534	-1.158657
27.C	1.745043	2.385540	0.717417
28.H	0.772255	0.998704	2.193905
29.C	1.745043	2.385540	-0.717417
30.H	0.772255	0.998704	-2.193905
31.H	2.265214	3.092977	1.357899
32.H	2.265214	3.092977	-1.357899
33.Fe	2.546147	0.615830	0.000000
34.XX	4.741423	-0.497199	0.000000
35.C	3.244399	-1.351145	0.000000
36.C	3.720255	-0.654739	-1.160255
37.C	3.720255	-0.654739	1.160255
38.H	2.611379	-2.234841	0.000000
39.C	4.495706	0.469861	-0.717442
40.H	3.523478	-0.927746	-2.193927
41.C	4.495706	0.469861	0.717442
42.H	3.523478	-0.927746	2.193927
43.H	4.987075	1.199494	-1.356249
44.H	4.987075	1.199494	1.356249

Symmetry A.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	2.4968	0.53675E-04	0.0000	0.0000	-0.29622E-01
2	2.5892	0.31240E-03	0.0000	0.0000	0.70177E-01
3	2.8373	0.23228E-04	0.0000	0.0000	0.18280E-01
5	3.0212	0.16478E-04	0.0000	0.0000	-0.14921E-01
6	3.4955	0.36355E-04	0.0000	0.0000	0.20604E-01
8	4.0704	0.13652E-02	0.0000	0.0000	-0.11700
9	4.3698	0.20881E-03	0.0000	0.0000	0.44164E-01

Major MO -> MO transitions for the above excitations

	Excit. No.	Occ.	to	vi	Contrib. sum=1)	transition moment x	y	z
1:	11b.g	->	18b.u		0.7244	0.0000	0.0000	-0.1283
1:	18a.g	->	12a.u		0.2351	0.0000	0.0000	0.0490
1:	11a.u	->	19a.g		0.0378	0.0000	0.0000	-0.0244
2:	18a.g	->	12a.u		0.5413	0.0000	0.0000	0.0730
2:	17b.u	->	12b.g		0.2331	0.0000	0.0000	0.0418
2:	11b.g	->	18b.u		0.1438	0.0000	0.0000	0.0561
2:	11a.u	->	19a.g		0.0655	0.0000	0.0000	0.0316
3:	17b.u	->	12b.g		0.5142	0.0000	0.0000	-0.0594
3:	11a.u	->	19a.g		0.3927	0.0000	0.0000	0.0739
3:	18a.g	->	12a.u		0.0652	0.0000	0.0000	0.0242
5:	16b.u	->	12b.g		0.3346	0.0000	0.0000	-0.0143
5:	11a.u	->	19a.g		0.2562	0.0000	0.0000	0.0578
5:	17a.g	->	12a.u		0.2509	0.0000	0.0000	0.0105
5:	17b.u	->	12b.g		0.0997	0.0000	0.0000	0.0253
6:	16b.u	->	12b.g		0.2618	0.0000	0.0000	-0.0118
6:	11a.u	->	19a.g		0.2221	0.0000	0.0000	-0.0501
6:	17b.u	->	12b.g		0.1365	0.0000	0.0000	-0.0276
6:	17a.g	->	12a.u		0.1242	0.0000	0.0000	0.0068
6:	18a.g	->	12a.u		0.1239	0.0000	0.0000	0.0301
6:	11b.g	->	18b.u		0.0953	0.0000	0.0000	0.0393
8:	11b.g	->	19b.u		0.9382	0.0000	0.0000	-0.4509
9:	10b.g	->	18b.u		0.9874	0.0000	0.0000	0.1887

Symmetry B.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	2.4977	0.45802E-01	0.86146	0.79965E-01	0.0000
2	2.6599	0.48599E-02	-0.27125	-0.31611E-01	0.0000
3	2.7518	0.39608E-02	-0.23905	-0.40027E-01	0.0000
4	2.8953	0.72400E-02	-0.31937	-0.85931E-02	0.0000
5	3.1612	0.28615E-02	0.19205	0.79891E-02	0.0000
6	3.5211	0.18975E-02	0.14706	0.19215E-01	0.0000
7	3.8422	0.45296E-01	0.69130	-0.57503E-01	0.0000
8	4.1345	0.24146	1.5351	0.16509	0.0000

Major MO -> MO transitions for the above excitations

	Excit. No.	Occ.	to	virt.	Contrib. (sum=1)	transition moment x	y	z
1:	18a.g	->	18b.u		0.8656	1.5685	-0.0219	0.0000
1:	11a.u	->	12b.g		0.0839	-0.0749	-0.0009	0.0000
2:	11b.g	->	12a.u		0.5557	-0.1601	-0.0036	0.0000
2:	11a.u	->	12b.g		0.4237	-0.1631	-0.0019	0.0000
3:	17a.g	->	18b.u		0.8914	-0.3585	-0.0023	0.0000
4:	17b.u	->	19a.g		0.4784	-0.6398	0.0896	0.0000
4:	11a.u	->	12b.g		0.2630	-0.1231	-0.0015	0.0000
4:	11b.g	->	12a.u		0.2233	0.0973	0.0022	0.0000
5:	16b.u	->	19a.g		0.7017	0.3883	-0.0125	0.0000
5:	17b.u	->	19a.g		0.1934	0.3893	-0.0545	0.0000
6:	17b.u	->	19a.g		0.2620	-0.4294	0.0601	0.0000
6:	16b.u	->	19a.g		0.2513	0.2202	-0.0071	0.0000
6:	11a.u	->	12b.g		0.1529	0.0851	0.0010	0.0000
6:	11b.g	->	12a.u		0.1458	-0.0713	-0.0016	0.0000
6:	17a.g	->	18b.u		0.0997	-0.1060	-0.0007	0.0000
6:	18a.g	->	18b.u		0.0662	0.3654	-0.0051	0.0000
7:	16a.g	->	18b.u		0.6435	2.2537	-0.5165	0.0000
7:	18a.g	->	19b.u		0.3273	-0.9871	-0.0160	0.0000
8:	18a.g	->	19b.u		0.5655	1.2507	0.0202	0.0000
8:	16a.g	->	18b.u		0.2495	1.3528	-0.3100	0.0000
8:	10a.u	->	12b.g		0.0498	-0.5299	0.3346	0.0000
8:	11a.u	->	13b.g		0.0481	-0.2118	0.2165	0.0000

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b) Fc2 calculated by Gaussian 03

6	-1.774065	2.979937	0.000000
6	-1.150152	3.565873	1.176953
6	-1.150152	3.565873	-1.176953

1	-2.547670	2.212332	0.000000
6	-0.143931	4.518022	0.727593
1	-1.390644	3.330188	2.213557
6	-0.143931	4.518022	-0.727593
1	-1.390644	3.330188	-2.213557
1	0.500730	5.119904	1.368366
1	0.500730	5.119904	-1.368366
26	0.283607	2.601189	0.000000
6	0.534366	0.500969	0.000000
6	1.150152	1.114074	-1.174801
6	1.150152	1.114074	1.174801
6	2.159756	2.058972	-0.727728
1	0.909238	0.883404	-2.212429
6	2.159756	2.058972	0.727728
1	0.909238	0.883404	2.212429
1	2.799057	2.663878	-1.370339
1	2.799057	2.663878	1.370339
6	-0.534366	-0.500969	0.000000
6	-1.150152	-1.114074	-1.174801
6	-1.150152	-1.114074	1.174801
6	-2.159756	-2.058972	-0.727728
1	-0.909238	-0.883404	-2.212429
6	-2.159756	-2.058972	0.727728
1	-0.909238	-0.883404	2.212429
1	-2.799057	-2.663878	-1.370339
1	-2.799057	-2.663878	1.370339
26	-0.283607	-2.601189	0.000000
6	1.774065	-2.979937	0.000000
6	1.150152	-3.565873	1.176953
6	1.150152	-3.565873	-1.176953
1	2.547670	-2.212332	0.000000
6	0.143931	-4.518022	0.727593
1	1.390644	-3.330188	2.213557
6	0.143931	-4.518022	-0.727593
1	1.390644	-3.330188	-2.213557
6	0.143931	-4.518022	-0.727593
1	1.390644	-3.330188	-2.213557
1	-0.500730	-5.119904	1.368366
1	-0.500730	-5.119904	-1.368366

Sum of electronic and zero-point Energies= -1019.636860
Sum of electronic and thermal Energies= -1019.618736
Sum of electronic and thermal Enthalpies= -1019.617791
Sum of electronic and thermal Free Energies=-1019.682211

Molecular orbitals involved in electronic excitations:

MO	symmetry
76	15bu
77	10bg
78	10au
79	16ag
80	16bu
81	17ag
82	17bu
83	11au
84	11bg
85	18ag
86	18bu
87	12au
88	12bg
89	19ag
90	19bu
93	13bg

Excitation energies and oscillator strengths: (Only allowed transitions)

Excited State 1: Singlet-BU 2.4008 eV f=0.0321
83 -> 88 -0.25109
84 -> 87 -0.19204
85 -> 86 0.61161

Excited State 3: Singlet-AU 2.4114 eV f=0.0001
82 -> 88 0.12918
84 -> 86 0.59762
85 -> 87 0.36969

Excited State 5: Singlet-AU 2.6265 eV f=0.0004
82 -> 88 -0.24082
83 -> 89 0.24000
84 -> 86 -0.27712
85 -> 87 0.53529

Excited State 8: Singlet-BU 2.6975 eV f=0.0002
81 -> 86 -0.10082
83 -> 88 -0.38558
84 -> 87 0.57915

Excited State 10: Singlet-BU 2.7375 eV f=0.0108
80 -> 89 0.12290
81 -> 86 0.52144
83 -> 88 -0.39523
84 -> 87 -0.15442
85 -> 86 -0.15164

Excited State 12: Singlet-AU 2.7623 eV f=0.0000
82 -> 88 0.55002
83 -> 89 0.42530
84 -> 86 -0.11030

Excited State 14: Singlet-BU 2.8511 eV f=0.0104
81 -> 86 -0.36875
82 -> 89 0.51773
83 -> 88 -0.20622
84 -> 87 -0.13156
85 -> 86 -0.15655

Excited State 16: Singlet-AU 2.9308 eV f=0.0000
80 -> 88 0.36215
81 -> 87 0.41988
82 -> 88 0.19604
83 -> 89 -0.38558
85 -> 87 0.10018

Excited State 18: Singlet-AU 3.0995 eV f=0.0000
80 -> 88 -0.48624
81 -> 87 0.50623

Excited State 20: Singlet-BU 3.1825 eV f=0.0040
80 -> 89 0.55545
81 -> 86 -0.21268
82 -> 89 -0.29507
83 -> 88 -0.13436
84 -> 87 -0.13760

Excited State 22: Singlet-AU 3.4825 eV f=0.0001
80 -> 88 0.33963
81 -> 87 0.23482
82 -> 88 -0.25311
83 -> 89 0.30089
84 -> 86 0.17374
85 -> 87 -0.20815

Excited State 24: Singlet-BU 3.5199 eV f=0.0020
80 -> 89 0.40907
81 -> 86 0.16455
82 -> 89 0.30715
83 -> 88 0.22995
84 -> 87 0.22069
85 -> 86 0.14439

Excited State 25: Singlet-BU 3.7959 eV f=0.0863
79 -> 86 0.58933
85 -> 90 -0.34446

Excited State 27: Singlet-AU 3.9213 eV f=0.0000
79 -> 87 0.69061

Excited State 28: Singlet-AU 4.0838 eV f=0.0015
84 -> 90 0.69564

Excited State 31: Singlet-BU 4.1410 eV f=0.1992
78 -> 88 -0.17273
79 -> 86 0.25890
83 -> 93 -0.13787
85 -> 90 0.55874

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2. Bisferrocene radical cation (Fc2.+)

a. calculated by ADF

1.XX	-4.741423	0.497199	0.000000
2.C	-3.424931	1.393979	0.000000
3.C	-3.842922	0.664556	-1.164441
4.C	-3.842922	0.664556	1.164441
5.H	-2.864804	2.326919	0.000000
6.C	-4.539460	-0.518756	-0.721400
7.H	-3.691887	0.968246	-2.197357
8.C	-4.539460	-0.518756	0.721400
9.H	-3.691887	0.968246	2.197357
10.H	-5.011519	-1.260192	-1.361567
11.H	-5.011519	-1.260192	1.361567
12.Fe	-2.572320	-0.579659	0.000000
13.XX	-1.039653	-1.729750	0.000000
14.C	-0.415899	-0.594530	0.000000
15.C	-0.957770	-1.260657	1.166945
16.C	-0.957770	-1.260657	-1.166945
17.C	-1.760943	-2.368954	0.720767
18.H	-0.752909	-1.006138	2.202657
19.C	-1.760943	-2.368954	-0.720767
20.H	-0.752909	-1.006138	-2.202657
21.H	-2.266007	-3.087008	1.361964
22.H	-2.266007	-3.087008	-1.361964
23.C	0.415899	0.594530	0.000000
24.XX	1.039653	1.729750	0.000000
25.C	0.957770	1.260657	1.166945
26.C	0.957770	1.260657	-1.166945
27.C	1.760943	2.368954	0.720767
28.H	0.752909	1.006138	2.202657
29.C	1.760943	2.368954	-0.720767

30.H	0.752909	1.006138	-2.202657
31.H	2.266007	3.087008	1.361964
32.H	2.266007	3.087008	-1.361964
33.Fe	2.572320	0.579659	0.000000
34.XX	4.741423	-0.497199	0.000000
35.C	3.424931	-1.393979	0.000000
36.C	3.842922	-0.664556	-1.164441
37.C	3.842922	-0.664556	1.164441
38.H	2.864804	-2.326919	0.000000
39.C	4.539460	0.518756	-0.721400
40.H	3.691887	-0.968246	-2.197357
41.C	4.539460	0.518756	0.721400
42.H	3.691887	-0.968246	2.197357
43.H	5.011519	1.260192	-1.361567
44.H	5.011519	1.260192	1.361567

Symmetry A.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
2	2.0344	0.11120E-02	0.0000	0.0000	0.14937
3	2.2540	0.16325E-04	0.0000	0.0000	0.17194E-01
4	2.3956	0.50014E-04	0.0000	0.0000	0.29192E-01
5	2.5293	0.24488E-04	0.0000	0.0000	-0.19879E-01
6	2.6121	0.15854E-03	0.0000	0.0000	-0.49773E-01
11	2.9911	0.38129E-04	0.0000	0.0000	0.22811E-01
12	3.0170	0.13159E-04	0.0000	0.0000	0.13343E-01
13	3.1269	0.15190E-04	0.0000	0.0000	0.14081E-01

Major MO -> MO transitions for the above excitations

Excit. No.	Occ.	to	virt.	Contrib. (sum=1)	transition moment x	y	z
2: Beta	10a.u	->	18a.g	0.9988	0.0000	0.0000	0.4529
3: Alph	11b.g	->	18b.u	0.5971	0.0000	0.0000	0.1026
3: Beta	11b.g	->	18b.u	0.3201	0.0000	0.0000	-0.0582
3: Beta	11a.u	->	19a.g	0.0480	0.0000	0.0000	0.0207
4: Beta	17b.u	->	12b.g	0.7558	0.0000	0.0000	0.0708
4: Alph	17a.g	->	12a.u	0.0534	0.0000	0.0000	0.0230
4: Alph	17b.u	->	12b.g	0.0454	0.0000	0.0000	-0.0015
5: Beta	17a.g	->	12a.u	0.2882	0.0000	0.0000	0.0153
5: Beta	16b.u	->	12b.g	0.2154	0.0000	0.0000	-0.0101
5: Alph	18a.g	->	12a.u	0.2093	0.0000	0.0000	-0.0184
5: Alph	17b.u	->	12b.g	0.1465	0.0000	0.0000	-0.0026
5: Beta	17b.u	->	12b.g	0.0481	0.0000	0.0000	-0.0174
6: Beta	11b.g	->	18b.u	0.4977	0.0000	0.0000	-0.0674
6: Alph	11b.g	->	18b.u	0.3029	0.0000	0.0000	-0.0679
6: Alph	11a.u	->	19a.g	0.0754	0.0000	0.0000	-0.0254
11: Alph	17a.g	->	12a.u	0.6060	0.0000	0.0000	0.0694
11: Beta	11a.u	->	19a.g	0.1021	0.0000	0.0000	0.0261
11: Alph	11a.u	->	19a.g	0.0981	0.0000	0.0000	0.0271
12: Alph	17b.u	->	12b.g	0.2426	0.0000	0.0000	0.0030
12: Alph	18a.g	->	12a.u	0.2008	0.0000	0.0000	0.0165
12: Beta	16b.u	->	12b.g	0.1999	0.0000	0.0000	-0.0089
12: Beta	17a.g	->	12a.u	0.1211	0.0000	0.0000	0.0091
12: Beta	11a.u	->	19a.g	0.0913	0.0000	0.0000	0.0246
12: Alph	11a.u	->	19a.g	0.0869	0.0000	0.0000	0.0254
13: Alph	16b.u	->	12b.g	0.5135	0.0000	0.0000	0.0345
13: Beta	11a.u	->	19a.g	0.1528	0.0000	0.0000	-0.0313
13: Alph	11a.u	->	19a.g	0.1506	0.0000	0.0000	-0.0328
13: Alph	17a.g	->	12a.u	0.1395	0.0000	0.0000	0.0326
14: Alph	16a.g	->	12a.u	0.4399	0.0000	0.0000	0.0595
14: Alph	16b.u	->	12b.g	0.2517	0.0000	0.0000	-0.0228
14: Beta	11a.u	->	19a.g	0.0633	0.0000	0.0000	-0.0190
14: Alph	11a.u	->	19a.g	0.0583	0.0000	0.0000	-0.0193
14: Alph	17a.g	->	12a.u	0.0528	0.0000	0.0000	0.0189

Symmetry B.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	0.66816	0.12800E-01	0.85973	0.20692	0.0000
2	0.83609	0.36502E-01	-1.2993	-0.30610	0.0000
4	2.3080	0.89541E-02	0.39420	-0.54434E-01	0.0000
5	2.4818	0.95945E-02	-0.39492	-0.42784E-01	0.0000
6	2.5000	0.22045E-03	0.59854E-01	0.40778E-02	0.0000
7	2.6152	0.34040E-01	0.72766	0.42318E-01	0.0000
8	2.6928	0.94088E-02	0.37751	0.10161E-01	0.0000
9	2.8153	0.15832E-02	-0.15093	-0.13204E-01	0.0000
10	2.8707	0.16267E-04	0.93594E-02	0.11987E-01	0.0000
11	2.8873	0.13634E-02	-0.13830	-0.12114E-01	0.0000
12	3.0496	0.19146E-02	0.15599	-0.35967E-01	0.0000
13	3.2231	0.36014E-01	0.66961	0.87768E-01	0.0000
14	3.2297	0.76901E-03	0.37991E-01	0.90969E-01	0.0000
15	3.3129	0.11532E-02	-0.10397	-0.58297E-01	0.0000
16	3.6114	0.11718	1.1504	0.29284E-01	0.0000

Major MO -> MO transitions for the above excitations

Excit. No.	Occ.	to	virt.	Contrib. (sum=1)	transition moment x	y	z
1: Beta	17b.u	->	18a.g	0.5215	2.0307	0.3980	0.0000
1: Beta	16b.u	->	18a.g	0.4722	-0.6430	-0.1049	0.0000
2: Beta	16b.u	->	18a.g	0.5212	-0.6040	-0.0985	0.0000
2: Beta	17b.u	->	18a.g	0.4530	-1.6918	-0.3316	0.0000
4: Beta	15b.u	->	18a.g	0.9388	0.4926	-0.3553	0.0000
5: Beta	17b.u	->	19a.g	0.5932	-0.5728	0.0223	0.0000
5: Alph	17a.g	->	18b.u	0.1784	-0.7401	0.0842	0.0000
5: Beta	17a.g	->	18b.u	0.0884	0.1468	-0.0166	0.0000
6: Alph	11a.u	->	12b.g	0.2798	0.1480	-0.0374	0.0000
6: Alph	11b.g	->	12a.u	0.2436	-0.0412	-0.0245	0.0000
6: Beta	11a.u	->	12b.g	0.2319	-0.1281	0.0303	0.0000
6: Beta	11b.g	->	12a.u	0.1995	0.0388	0.0226	0.0000
7: Alph	18a.g	->	18b.u	0.4402	0.5082	-0.0556	0.0000
7: Beta	17a.g	->	18b.u	0.3592	0.2883	-0.0327	0.0000
7: Alph	17a.g	->	18b.u	0.0964	0.5300	-0.0603	0.0000
8: Alph	17a.g	->	18b.u	0.5896	1.2915	-0.1470	0.0000
8: Beta	17b.u	->	19a.g	0.2383	-0.3485	0.0136	0.0000
9: Alph	11b.g	->	12a.u	0.5152	-0.0564	-0.0335	0.0000
9: Alph	11a.u	->	12b.g	0.4749	-0.1816	0.0460	0.0000
10: Beta	16b.u	->	19a.g	0.6473	0.2697	0.0617	0.0000
10: Alph	17b.u	->	19a.g	0.2524	-0.0119	-0.0481	0.0000
11: Beta	11b.g	->	12a.u	0.5163	-0.0581	-0.0338	0.0000
11: Beta	11a.u	->	12b.g	0.4732	-0.1703	0.0403	0.0000
12: Alph	17b.u	->	19a.g	0.4640	-0.0157	-0.0633	0.0000
12: Beta	16b.u	->	19a.g	0.1464	-0.1244	-0.0285	0.0000
12: Beta	11b.g	->	12a.u	0.0989	-0.0248	-0.0144	0.0000
12: Beta	11a.u	->	12b.g	0.0973	0.0751	-0.0178	0.0000
12: Alph	11b.g	->	12a.u	0.0830	-0.0218	-0.0129	0.0000
12: Alph	11a.u	->	12b.g	0.0771	0.0703	-0.0178	0.0000
13: Alph	16a.g	->	18b.u	0.5069	1.4177	-0.3007	0.0000
13: Beta	14b.u	->	18a.g	0.2236	0.1846	0.1219	0.0000
13: Beta	16a.g	->	18b.u	0.2202	-0.9901	0.2572	0.0000
14: Beta	14b.u	->	18a.g	0.6345	0.3107	0.2051	0.0000
14: Alph	16a.g	->	18b.u	0.2040	-0.8984	0.1906	0.0000
15: Alph	16b.u	->	19a.g	0.7009	-0.4262	0.0303	0.0000
15: Beta	16b.u	->	19a.g	0.0637	-0.0787	-0.0180	0.0000
15: Alph	17b.u	->	19a.g	0.0484	-0.0049	-0.0196	0.0000
16: Beta	16a.g	->	18b.u	0.4038	1.2667	-0.3290	0.0000
16: Beta	14b.u	->	18a.g	0.0720	0.0990	0.0653	0.0000
16: Alph	17b.u	->	19a.g	0.0719	0.0057	0.0229	0.0000
16: Alph	16a.g	->	18b.u	0.0633	0.4732	-0.1004	0.0000
16: Alph	17a.g	->	18b.u	0.0564	0.3450	-0.0393	0.0000
16: Beta	11a.u	->	12b.g	0.0536	0.0513	-0.0121	0.0000
16: Alph	11a.u	->	12b.g	0.0476	0.0508	-0.0128	0.0000
16: Beta	11b.g	->	12a.u	0.0454	-0.0154	-0.0090	0.0000

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b) Fc2.+ calculated by Gaussian 03

6	-1.813757	3.234411	0.000000
6	-1.136629	3.745225	1.174816
6	-1.136629	3.745225	-1.174816
1	-2.662057	2.549133	0.000000
6	-0.043377	4.594789	0.727411
1	-1.408291	3.544080	2.210703
6	-0.043377	4.594789	-0.727411
1	-1.408291	3.544080	-2.210703
1	0.644551	5.145510	1.368385
1	0.644551	5.145510	-1.368385
26	0.262207	2.641295	0.000000
6	0.543573	0.485492	0.000000
6	1.136629	1.119998	-1.175444
6	1.136629	1.119998	1.175444
6	2.143047	2.062987	-0.726803
1	0.906161	0.884978	-2.214058
6	2.143047	2.062987	0.726803
1	0.906161	0.884978	2.214058
1	2.787278	2.662181	-1.368961
1	2.787278	2.662181	1.368961
6	-0.543573	-0.485492	0.000000
6	-1.136629	-1.119998	-1.175444
6	-1.136629	-1.119998	1.175444

6	-2.143047	-2.062987	-0.726803
1	-0.906161	-0.884978	-2.214058
6	-2.143047	-2.062987	0.726803
1	-0.906161	-0.884978	2.214058
1	-2.787278	-2.662181	-1.368961
1	-2.787278	-2.662181	1.368961
26	-0.262207	-2.641295	0.000000
6	1.813757	-3.234411	0.000000
6	1.136629	-3.745225	1.174816
6	1.136629	-3.745225	-1.174816
1	2.662057	-2.549133	0.000000
6	0.043377	-4.594789	0.727411
1	1.408291	-3.544080	2.210703
6	0.043377	-4.594789	-0.727411
1	1.408291	-3.544080	-2.210703
1	-0.644551	-5.145510	1.368385
1	-0.644551	-5.145510	-1.368385

Sum of electronic and zero-point Energies= -1019.417622
Sum of electronic and thermal Energies= -1019.399026
Sum of electronic and thermal Enthalpies= -1019.398082
Sum of electronic and thermal Free Energies= -1019.466141

Molecular orbitals involved in electronic excitations:

MO	symmetry
76	15bu
77	10bg
78	10au
79	16ag
80	16bu
81	17ag
82	17bu
83	11au
84	11bg
85	18ag
86	18bu
87	12au
88	12bg
89	19ag
90	19bu
93	13bg

Excitation energies and oscillator strengths: (Only allowed transitions)

Excited State 1: ?Spin -AU 0.4676 eV f=0.0000
81B -> 85B 1.34873
82B -> 86B 0.11799

Excited State 3: ?Spin -BU 0.6520 eV f=0.0419
75A -> 86A -0.10113
81A -> 86A -0.15380
81A -> 90A -0.10939
83A -> 86A 0.12294
80B -> 85B 0.26935
84B -> 85B 0.65543

Excited State 5: ?Spin -BU 0.8291 eV f=0.0079
83A -> 86A -0.13423
80B -> 85B 1.01252
84B -> 85B -0.13110

Excited State 9: ?Spin -AU 1.8889 eV f=0.0000
79A -> 88A -0.10914
80A -> 87A -0.19497
81A -> 88A 0.19502
82A -> 87A 0.10434
84A -> 89A 0.33085
85A -> 86A 0.66306
74B -> 85B -0.21599
78B -> 85B 0.11375
81B -> 89B -0.36851
82B -> 86B -0.56667
84B -> 87B -0.45471

Excited State 10: ?Spin -BU 1.9788 eV f=0.0002
81A -> 86A -0.35270
82A -> 89A -0.33316
83A -> 86A -0.52275
84A -> 87A 0.29213
85A -> 88A 0.28142
80B -> 89B 0.35764
81B -> 87B -0.27984
82B -> 88B -0.27360
83B -> 86B 0.61364
84B -> 89B 0.21276

Excited State 12: ?Spin -AU 2.0369 eV f=0.0011
81A -> 88A 0.12301
82A -> 87A 0.15848
83A -> 88A 0.10011
84A -> 89A -0.10873
85A -> 86A -0.23469
78B -> 85B 0.89680
80B -> 87B -0.15527
82B -> 86B 0.14075
83B -> 88B -0.17486
84B -> 87B -0.23709

Excited State 13: ?Spin -BU 2.0452 eV f=0.0167
79A -> 86A 0.22966
80A -> 89A 0.28862
81A -> 86A -0.21118
83A -> 86A 0.34071
84A -> 87A 0.29735
85A -> 88A 0.27262
72B -> 85B -0.15837
76B -> 85B -0.41916
80B -> 89B -0.22571
81B -> 87B -0.27322
82B -> 88B -0.27858
83B -> 86B -0.37263
84B -> 89B 0.55139

Excited State 15: ?Spin -AU 2.0597 eV f=0.0001
81A -> 88A -0.29022
82A -> 87A -0.38122
83A -> 88A -0.24571
84A -> 89A 0.12039
85A -> 86A 0.29419
74B -> 85B 0.19766
78B -> 85B 0.42588
80B -> 87B 0.35205
82B -> 86B -0.16013
83B -> 88B 0.40374
84B -> 87B 0.58250

Excited State 18: ?Spin -BU 2.2613 eV f=0.0035
81A -> 86A 0.15940
82A -> 89A 0.10402
83A -> 86A 0.22903
84A -> 87A 0.45249
85A -> 88A 0.44784
76B -> 85B 0.56494
81B -> 87B -0.33914
82B -> 88B -0.32600
83B -> 86B -0.11896
84B -> 89B -0.33745

Excited State 19: ?Spin -AU 2.2880 eV f=0.0000
79A -> 88A 0.14666
80A -> 87A 0.25122
82A -> 87A 0.33697
83A -> 88A 0.41860
85A -> 86A 0.35282
74B -> 85B 0.23686
80B -> 87B -0.46075
83B -> 88B -0.44809
84B -> 87B 0.50530

Excited State 21: ?Spin -BU 2.3665 eV f=0.0010
80A -> 89A 0.11944
81A -> 86A -0.17827
84A -> 87A -0.13764
85A -> 88A -0.14941
76B -> 85B 0.70627
81B -> 87B 0.12732
82B -> 88B 0.12220
84B -> 89B 0.63166

Excited State 23: ?Spin -AU 2.5897 eV f=0.0001
80A -> 87A -0.21076
81A -> 88A 0.15222
83A -> 88A -0.23104
84A -> 89A -0.22892
85A -> 86A 0.54449
74B -> 85B 0.15851
82B -> 86B 0.70220
84B -> 87B -0.12853

Excited State 25: ?Spin -BU 2.5970 eV f=0.0343
79A -> 86A 0.16149
80A -> 89A 0.12435
81A -> 86A -0.58841
83A -> 86A 0.57154
79B -> 86B 0.17674
80B -> 89B 0.11941
81B -> 87B 0.17939
82B -> 88B 0.13860
83B -> 86B 0.32826
84B -> 89B -0.29572

Excited State 26: ?Spin -AU 2.6335 eV f=0.0000
80A -> 87A 0.12601
81A -> 88A -0.18491
83A -> 88A 0.10221
74B -> 85B 0.87468
82B -> 86B -0.14273
84B -> 87B -0.39905

Excited State 27: ?Spin -BU 2.6494 eV f=0.0030
81A -> 86A 0.54168

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     83A -> 86A        0.41552
     84A -> 87A       -0.17734
     85A -> 88A       -0.18531
     81B -> 87B       -0.24969
     82B -> 88B       -0.24171
     83B -> 86B        0.56014
     84B -> 89B        0.17939


Excited State  31:   ?Spin  -AU     2.8415 eV  f=0.0000
     80A -> 87A       -0.11515
     81A -> 88A        0.22177
     82A -> 87A        0.13159
     84A -> 89A        0.76366
     85A -> 86A       -0.22068
     74B -> 85B        0.14681
     81B -> 89B       -0.39827
     82B -> 86B        0.34522

Excited State  34:   ?Spin  -BU     2.8520 eV  f=0.0006
     84A -> 87A       -0.70253
     85A -> 88A        0.70924

 Excited State  35:   ?Spin  -BU     2.9171 eV  f=0.0050
     79A -> 86A       -0.38103
     80A -> 89A       -0.19607
     82A -> 89A       -0.26718
     83A -> 86A        0.23712
     84A -> 87A       -0.10013
     85A -> 88A       -0.10886
     79B -> 86B        0.24000
     80B -> 89B        0.70122
     82B -> 88B       -0.13243
     83B -> 86B       -0.33066
     84B -> 89B        0.10634


Excited State  38:   ?Spin  -AU     2.9211 eV  f=0.0000
     80A -> 87A       -0.15877
     81A -> 88A        0.52947
     82A -> 87A        0.52566
     83A -> 88A        0.11040
     74B -> 85B        0.16890
     80B -> 87B        0.32640
     81B -> 89B        0.33386
     82B -> 86B       -0.15429
     83B -> 88B        0.38807
     84B -> 87B        0.12259


Excited State  40:   ?Spin  -AU     2.9835 eV  f=0.0001
     83A -> 88A       -0.55110
     84A -> 89A        0.32557
     80B -> 87B       -0.11396
     81B -> 89B        0.63371
     82B -> 86B       -0.16566
     83B -> 88B       -0.36464

 Excited State  41:   ?Spin  -BU     3.0222 eV  f=0.0000
     82A -> 89A       -0.12606
     81B -> 87B       -0.64396
     82B -> 88B        0.73904

Excited State  43:   ?Spin  -AU     3.0328 eV  f=0.0000
     83A -> 88A        0.18841
     80B -> 87B        0.73366
     83B -> 88B       -0.62791

Excited State  45:   ?Spin  -BU     3.0460 eV  f=0.0043
     79A -> 86A       -0.23708
     80A -> 89A       -0.12394
     81A -> 86A       -0.26413
     82A -> 89A        0.70340
     84A -> 87A       -0.23058
     85A -> 88A       -0.22660
     72B -> 85B       -0.13850
     79B -> 86B        0.14961
     81B -> 87B       -0.41680
     82B -> 88B       -0.16870

Excited State  47:   ?Spin  -AU     3.0563 eV  f=0.0000
     80A -> 87A        0.13299
     81A -> 88A       -0.44369
     82A -> 87A        0.67997
     83A -> 88A       -0.47960
     84A -> 89A       -0.13702
     80B -> 87B        0.14300
     81B -> 89B       -0.21136

Excited State  50:   ?Spin  -BU     3.1133 eV  f=0.0234
     79A -> 86A        0.66049
     82A -> 89A        0.20689
     79B -> 86B       -0.43055
     80B -> 89B        0.51854
     82B -> 88B       -0.15755
     83B -> 86B       -0.10796

 Excited State  51:   ?Spin  -AU     3.1629 eV  f=0.0000
     79A -> 88A        0.15571
     80A -> 87A        0.61621
     81A -> 88A        0.55671
     82A -> 87A       -0.15275
     83A -> 88A       -0.34606
     84A -> 89A       -0.21147
     81B -> 89B       -0.28201

Excited State  53:   ?Spin  -BU     3.1804 eV  f=0.0097
     82A -> 89A        0.30083
     72B -> 85B        0.90658
     79B -> 86B        0.11775
     80B -> 89B        0.10910
     84B -> 89B        0.11638

 Excited State  54:   ?Spin  -BU     3.3291 eV  f=0.0004
     79A -> 86A       -0.36164
     80A -> 89A        0.80243
     82A -> 89A        0.20934
     72B -> 85B       -0.13560
     75B -> 86B       -0.13748
     79B -> 86B       -0.15718
     80B -> 89B        0.25527

Excited State  58:   ?Spin  -AU     3.4912 eV  f=0.0000
     79A -> 88A        0.73799
     80A -> 87A       -0.54058
     83A -> 88A       -0.12471
     84A -> 89A       -0.15932
     81B -> 89B       -0.18659

 Excited State  59:   ?Spin  -BU     3.4986 eV  f=0.0582
     72A -> 89A       -0.15507
     73A -> 88A        0.19769
     74A -> 87A        0.21178
     75A -> 86A        0.56684
     76A -> 89A       -0.19433
     79A -> 86A       -0.19603
     80A -> 89A       -0.18709
     81A -> 86A       -0.17981
     82A -> 89A       -0.13413
     83A -> 86A        0.10139
     72B -> 89B        0.11089
     73B -> 88B       -0.15123
     74B -> 87B       -0.16461
     75B -> 86B       -0.41368
     76B -> 89B        0.26408
     77B -> 88B        0.13949
     78B -> 87B        0.12585
     79B -> 86B       -0.32029
     82B -> 88B       -0.10358

 Excited State  60:   ?Spin  -AU     3.5135 eV f=0.0003
     77A -> 86A        0.97921
     77B -> 86B       -0.12003


Excited State  62:   ?Spin  -BU    3.5783 eV  nm  f=0.1250
     74A -> 87A        0.10226
     75A -> 86A        0.21021
     76A -> 89A       -0.16210
     77A -> 88A       -0.23528
     78A -> 87A       -0.31942
     79A -> 86A        0.22490
     81A -> 86A        0.10488
     82A -> 89A        0.10328
     72B -> 85B       -0.19636
     73B -> 88B       -0.15622
     74B -> 87B       -0.17650
     75B -> 86B       -0.30257
     76B -> 89B        0.13199
     79B -> 86B        0.66576

-----------------------------------------------------

3. bisfulvalenide (Fc=Fc)

a. calculated by ADF

    1.XX       -2.162155   -2.015309    0.000000
    2.C        -1.664655   -0.737453    0.000000
    3.C        -1.674161   -1.596846   -1.158386
    4.C        -1.698418   -2.961810   -0.716896
    5.C        -1.698418   -2.961810    0.716896
    6.C        -1.674161   -1.596846    1.158386
    7.H        -1.664570   -1.266815   -2.193828
    8.H        -1.707014   -3.839561   -1.357346
    9.H        -1.707014   -3.839561    1.357346
   10.H        -1.664570   -1.266815    2.193828
   11.Fe        0.000000   -2.003066    0.000000
   12.XX        2.162155   -2.015309    0.000000
   13.C         1.664655   -0.737453    0.000000
   14.C         1.674161   -1.596846    1.158386
   15.C         1.674161   -1.596846   -1.158386
   16.C         1.698418   -2.961810    0.716896
   17.H         1.664570   -1.266815    2.193828
```

18.C	1.698418	-2.961810	-0.716896
19.H	1.664570	-1.266815	-2.193828
20.H	1.707014	-3.839561	1.357346
21.H	1.707014	-3.839561	-1.357346
22.C	-1.664655	0.737453	0.000000
23.XX	-2.162155	2.015309	0.000000
24.C	-1.674161	1.596846	1.158386
25.C	-1.674161	1.596846	-1.158386
26.C	-1.698418	2.961810	0.716896
27.H	-1.664570	1.266815	2.193828
28.C	-1.698418	2.961810	-0.716896
29.H	-1.664570	1.266815	-2.193828
30.H	-1.707014	3.839561	1.357346
31.H	-1.707014	3.839561	-1.357346
32.Fe	0.000000	2.003066	0.000000
33.XX	2.162155	2.015309	0.000000
34.C	1.664655	0.737453	0.000000
35.C	1.674161	1.596846	-1.158386
36.C	1.674161	1.596846	1.158386
37.C	1.698418	2.961810	-0.716896
38.H	1.664570	1.266815	-2.193828
39.C	1.698418	2.961810	0.716896
40.H	1.664570	1.266815	2.193828
41.H	1.707014	3.839561	-1.357346
42.H	1.707014	3.839561	1.357346

Symmetry B1.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	4.2088	0.18621E-02	0.0000	0.0000	-0.13438
2	4.5414	0.29582E-03	0.0000	0.0000	0.51563E-01
3	4.6508	0.46746E-03	0.0000	0.0000	0.64052E-01
4	4.6565	0.67881E-03	0.0000	0.0000	-0.77138E-01
5	4.6895	0.69302E-03	0.0000	0.0000	0.77666E-01
6	4.8416	0.46312E-02	0.0000	0.0000	-0.19759
7	4.8714	0.84324E-03	0.0000	0.0000	-0.84056E-01
8	5.0474	0.44401E-02	0.0000	0.0000	-0.18949
9	5.0486	0.12196E-02	0.0000	0.0000	0.99299E-01
10	5.1235	0.67039E-03	0.0000	0.0000	-0.73080E-01
11	5.2195	0.79479E-02	0.0000	0.0000	0.24931
12	5.3238	0.19165E-03	0.0000	0.0000	-0.38333E-01
13	5.3737	0.13138E-02	0.0000	0.0000	0.99898E-01
14	5.4357	0.10151E-02	0.0000	0.0000	-0.87309E-01
15	5.6482	0.65444E-03	0.0000	0.0000	-0.68770E-01

Major MO -> MO transitions for the above excitations

Excit. No.	Occ.		to virt.	Contrib. (sum=1)	transition moment x	y	z
1:	6b1.u	->	11a.g	0.9901	0.0000	0.0000	-0.5630
2:	6b1.u	->	12a.g	0.9953	0.0000	0.0000	0.1684
3:	5b2.g	->	9b3.g	0.6076	0.0000	0.0000	0.3620
3:	6b3.g	->	10b2.u	0.3289	0.0000	0.0000	-0.0229
3:	7b1.g	->	6a.g	0.0508	0.0000	0.0000	0.0488
4:	6b3.g	->	10b2.u	0.6663	0.0000	0.0000	-0.0325
4:	5b2.g	->	9b3.g	0.2885	0.0000	0.0000	-0.2493
5:	9b2.u	->	7b3.g	0.9803	0.0000	0.0000	0.1276
6:	10a.g	->	7b1.g	0.9184	0.0000	0.0000	-0.7895
7:	7b1.g	->	6a.g	0.7702	0.0000	0.0000	-0.1856
7:	9a.g	->	7b1.g	0.1012	0.0000	0.0000	-0.0933
7:	10a.g	->	7b1.g	0.0485	0.0000	0.0000	-0.1809
8:	10a.g	->	8b1.g	0.9422	0.0000	0.0000	-0.2630
9:	9a.g	->	7b1.g	0.7594	0.0000	0.0000	0.2511
9:	8b2.u	->	7b3.g	0.0659	0.0000	0.0000	0.0671
9:	7b1.g	->	6a.g	0.0537	0.0000	0.0000	-0.0481
9:	10a.g	->	8b1.g	0.0533	0.0000	0.0000	-0.0625
10:	9b2.u	->	8b3.g	0.9942	0.0000	0.0000	-0.0601
11:	9a.g	->	8b1.g	0.9742	0.0000	0.0000	0.2773
12:	6b1.u	->	13a.g	0.9973	0.0000	0.0000	-0.1255
13:	8b2.u	->	7b3.g	0.7622	0.0000	0.0000	0.2213
13:	5a.u	->	8b1.g	0.1471	0.0000	0.0000	-0.1359
14:	8b3.u	->	6b2.g	0.5816	0.0000	0.0000	-0.2066
14:	5a.u	->	8b1.g	0.4029	0.0000	0.0000	-0.2236
15:	5a.u	->	8b1.g	0.3469	0.0000	0.0000	-0.2036
15:	8b3.u	->	6b2.g	0.3021	0.0000	0.0000	0.1460
15:	8b2.u	->	8b3.g	0.1203	0.0000	0.0000	-0.0639
15:	8b2.u	->	7b3.g	0.0968	0.0000	0.0000	-0.0769

Symmetry B2.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	3.9761	0.24132E-01	0.0000	-0.49773	0.0000
2	4.1690	0.53187E-02	0.0000	0.22820	0.0000
3	4.4595	0.21872E-01	0.0000	-0.44743	0.0000
4	4.6358	0.35522E-01	0.0000	0.55926	0.0000
5	4.7649	0.15406E-01	0.0000	-0.36328	0.0000
6	4.8066	0.24328E-01	0.0000	0.45452	0.0000
7	4.8569	0.21099E-01	0.0000	-0.42109	0.0000
8	4.8787	0.75821E-02	0.0000	0.25186	0.0000
9	4.9347	0.13843E-01	0.0000	0.33838	0.0000
10	5.0475	0.16480E-02	0.0000	0.11544	0.0000
11	5.0709	0.18809E-02	0.0000	0.12304	0.0000
12	5.2874	0.16533	0.0000	-1.1297	0.0000

Major MO -> MO transitions for the above excitations

Excit. No.	Occ.		to virt.	Contrib. (sum=1)	transition moment x	y	z
1:	9b2.u	->	11a.g	0.6834	0.0000	-1.4895	0.0000
1:	9b2.u	->	12a.g	0.2015	0.0000	0.3104	0.0000
1:	7b1.g	->	9b3.u	0.0843	0.0000	0.5025	0.0000
2:	9b2.u	->	12a.g	0.7464	0.0000	0.5835	0.0000
2:	7b1.g	->	9b3.u	0.1237	0.0000	-0.5945	0.0000
2:	9b2.u	->	11a.g	0.0983	0.0000	0.5517	0.0000
3:	8b2.u	->	11a.g	0.7844	0.0000	0.0394	0.0000
3:	7b1.g	->	9b3.u	0.0706	0.0000	-0.4341	0.0000
3:	6b3.g	->	7b1.u	0.0640	0.0000	-0.0852	0.0000
4:	6b3.g	->	7b1.u	0.5131	0.0000	0.2367	0.0000
4:	7b1.g	->	9b3.u	0.2701	0.0000	0.8328	0.0000
4:	8b2.u	->	11a.g	0.1441	0.0000	0.0166	0.0000
5:	8b2.u	->	12a.g	0.9644	0.0000	-0.1398	0.0000
6:	6b3.g	->	8b1.u	0.6094	0.0000	0.0380	0.0000
6:	7b1.g	->	9b3.u	0.1040	0.0000	0.5075	0.0000
6:	6b3.g	->	7b1.u	0.0835	0.0000	-0.0938	0.0000
6:	9b2.u	->	13a.g	0.0576	0.0000	-0.0100	0.0000
7:	6b3.g	->	8b1.u	0.3406	0.0000	0.0282	0.0000
7:	9b2.u	->	13a.g	0.2108	0.0000	0.0191	0.0000
7:	10a.g	->	10b2.u	0.1402	0.0000	0.0432	0.0000
7:	6b1.u	->	7b3.g	0.0855	0.0000	-0.2284	0.0000
7:	6b3.g	->	7b1.u	0.0819	0.0000	0.0924	0.0000
7:	7b1.g	->	9b3.u	0.0557	0.0000	-0.3696	0.0000
8:	10a.g	->	10b2.u	0.8053	0.0000	0.1034	0.0000
8:	9b2.u	->	13a.g	0.1509	0.0000	-0.0161	0.0000
9:	9b2.u	->	13a.g	0.5587	0.0000	0.0308	0.0000
9:	6b1.u	->	7b3.g	0.1311	0.0000	0.2806	0.0000
9:	5a.u	->	6b2.g	0.0731	0.0000	-0.0231	0.0000
9:	7b1.g	->	9b3.u	0.0531	0.0000	0.3579	0.0000
10:	9a.g	->	10b2.u	0.7773	0.0000	0.0225	0.0000
10:	5a.u	->	6b2.g	0.1667	0.0000	0.0346	0.0000
10:	5b2.g	->	6a.u	0.0485	0.0000	0.0095	0.0000
11:	5a.u	->	6b2.g	0.4259	0.0000	0.0551	0.0000
11:	5b2.g	->	6a.u	0.2293	0.0000	0.0206	0.0000
11:	9a.g	->	10b2.u	0.1796	0.0000	-0.0108	0.0000
11:	6b1.u	->	7b3.g	0.1124	0.0000	0.2563	0.0000
12:	7b2.u	->	11a.g	0.7897	0.0000	-1.6472	0.0000
12:	7b2.u	->	12a.g	0.0891	0.0000	0.1991	0.0000

Symmetry B3.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
2	2.4828	0.25182E-03	0.64342E-01	0.0000	0.0000
4	2.7615	0.12395E-02	0.13535	0.0000	0.0000
5	3.1267	0.41356E-03	-0.73476E-01	0.0000	0.0000
6	3.5926	0.67553E-03	0.87607E-01	0.0000	0.0000
7	4.1153	0.31278E-02	0.17613	0.0000	0.0000
8	4.2873	0.13448E-01	-0.35781	0.0000	0.0000
9	4.3249	0.10279E-03	-0.31146E-01	0.0000	0.0000
10	4.5475	0.20970E-04	-0.13719E-01	0.0000	0.0000
11	4.7167	0.44817E-02	-0.19693	0.0000	0.0000
12	4.8186	0.13249E-01	-0.33500	0.0000	0.0000
13	5.0017	0.93677E-02	-0.27649	0.0000	0.0000
14	5.3148	0.12953E-02	0.99738E-01	0.0000	0.0000
15	5.4829	0.10221E-01	0.27585	0.0000	0.0000

```
 16  5.6356      0.29679E-01  0.46364       0.0000  0.0000
```

Major MO -> MO transitions for the above excitations

```
 Excit. Occ. to    virt.     Contrib.   transition moment
  No.                        (sum=1)    x       y       z

 2: 9a.g   ->  9b3.u        0.9239  0.1123  0.0000  0.0000

 4: 9b2.u  ->  8b1.g        0.6823  0.4304  0.0000  0.0000
 4: 6b3.g  ->  6a.u         0.1679  0.0127  0.0000  0.0000
 4: 6b1.u  ->  6b2.g        0.1324  0.0293  0.0000  0.0000

 5: 8b2.u  ->  8b1.g        0.2833 -0.1193  0.0000  0.0000
 5: 6b3.g  ->  6a.u         0.2493  0.0146  0.0000  0.0000
 5: 6b1.u  ->  6b2.g        0.2243  0.0359  0.0000  0.0000
 5: 9b2.u  ->  8b1.g        0.1758 -0.2053  0.0000  0.0000
 5: 10a.g  ->  9b3.u        0.0574 -0.0502  0.0000  0.0000

 6: 8b2.u  ->  8b1.g        0.6920 -0.1739  0.0000  0.0000
 6: 6b3.g  ->  6a.u         0.0815 -0.0078  0.0000  0.0000
 6: 6b1.u  ->  6b2.g        0.0751 -0.0194  0.0000  0.0000
 6: 9b2.u  ->  8b1.g        0.0588  0.1108  0.0000  0.0000

 7: 7b2.u  ->  8b1.g        0.6140  2.2220  0.0000  0.0000
 7: 10a.g  ->  10b3.u       0.3665 -1.2470  0.0000  0.0000

 8: 10a.g  ->  10b3.u       0.5225 -1.4588  0.0000  0.0000
 8: 7b2.u  ->  8b1.g        0.2446 -1.3742  0.0000  0.0000
 8: 5b3.g  ->  6a.u         0.0994  0.8523  0.0000  0.0000
 8: 5b1.u  ->  6b2.g        0.0643  0.6884  0.0000  0.0000

 9: 9a.g   ->  10b3.u       0.9883 -0.3613  0.0000  0.0000

10: 5b3.g  ->  6a.u         0.5231 -1.8986  0.0000  0.0000
10: 5b1.u  ->  6b2.g        0.4698  1.8067  0.0000  0.0000

11: 6b1.u  ->  7b2.g        0.6941  1.5620  0.0000  0.0000
11: 5b1.u  ->  6b2.g        0.1822 -1.1047  0.0000  0.0000
11: 5b3.g  ->  6a.u         0.1056 -0.8378  0.0000  0.0000

12: 6b3.g  ->  7a.u         0.6845  1.4572  0.0000  0.0000
12: 6b1.u  ->  7b2.g        0.1128 -0.6229  0.0000  0.0000
12: 5b1.u  ->  6b2.g        0.0825 -0.7355  0.0000  0.0000
12: 5b3.g  ->  6a.u         0.0680 -0.6650  0.0000  0.0000

13: 8a.g   ->  9b3.u        0.7250  1.8611  0.0000  0.0000
13: 6b3.g  ->  7a.u         0.1620 -0.6957  0.0000  0.0000

14: 9b2.u  ->  9b1.g        0.9988 -0.0219  0.0000  0.0000

15: 10a.g  ->  11b3.u       0.9906 -0.0525  0.0000  0.0000

16: 9a.g   ->  11b3.u       0.9092 -0.5224  0.0000  0.0000
```

---

b) Fc=Fc calculated by Gaussian 03

```
  6          0.737443    1.682401    0.000000
  6          1.603847    1.678578    1.174590
  6          2.987877    1.691850    0.727269
  6          2.987877    1.691850   -0.727269
  6          1.603847    1.678578   -1.174590
  1          1.270225    1.681336    2.212084
  1          3.867953    1.700401    1.370117
  1          3.867953    1.700401   -1.370117
  1          1.270225    1.681336   -2.212084
 26          2.000365    0.000000    0.000000
  6          0.737443   -1.682401    0.000000
  6          1.603847   -1.678578   -1.174590
  6          1.603847   -1.678578    1.174590
  6          2.987877   -1.691850   -0.727269
  1          1.270225   -1.681336   -2.212084
  6          2.987877   -1.691850    0.727269
  1          1.270225   -1.681336    2.212084
  1          3.867953   -1.700401   -1.370117
  1          3.867953   -1.700401    1.370117
  6         -0.737443    1.682401    0.000000
  6         -1.603847    1.678578   -1.174590
  6         -1.603847    1.678578    1.174590
  6         -2.987877    1.691850   -0.727269
  1         -1.270225    1.681336   -2.212084
  6         -2.987877    1.691850    0.727269
  1         -1.270225    1.681336    2.212084
  1         -3.867953    1.700401   -1.370117
  1         -3.867953    1.700401    1.370117
 26         -2.000365    0.000000    0.000000
  6         -0.737443   -1.682401    0.000000
  6         -1.603847   -1.678578    1.174590
  6         -1.603847   -1.678578   -1.174590
  6         -2.987877   -1.691850    0.727269
  1         -1.270225   -1.681336    2.212084
  6         -2.987877   -1.691850   -0.727269
  1         -1.270225   -1.681336   -2.212084
  1         -3.867953   -1.700401    1.370117
```

```
  1         -3.867953   -1.700401   -1.370117

Sum of electronic and zero-point Energies=   -1018.465060
Sum of electronic and thermal Energies=      -1018.447861
Sum of electronic and thermal Enthalpies=    -1018.446917
Sum of electronic and thermal Free Energies= -1018.506892
```

Molecular orbitals involved in electronic excitations:

```
MO  symmetry
71   8ag
73   5b2g
74   5au
75   7b1g
76   5b1u
77   5b3g
78   7b2u
79   9ag
80   8b2u
81   10ag
82   6b1u
83   6b3g
84   9b2u
85   9b3u
86   6b2g
87   6au
88   8b1g
89   10b3u
90   11ag
91   10b2u
92   7b1u
93   7b2g
94   8b1u
95   12ag
96   7b3g
97   11b3u
98   7au
99   8b3g
100  9b1g
101  13ag
```

Excitation energies and oscillator strengths: (Only allowed transitions)

```
Excited State   4:   Singlet-B2U     2.2504 eV    f=0.0000
      79 -> 85        -0.12032
      81 -> 85         0.65669
      82 -> 86         0.16877
      83 -> 87         0.17337

Excited State   7:   Singlet-B2U     2.4889 eV    f=0.0001
      79 -> 85         0.67641
      82 -> 86         0.13554
      83 -> 87         0.13924
      84 -> 88        -0.11213

Excited State   9:   Singlet-B2U     2.6359 eV    f=0.0013
      82 -> 86         0.25075
      83 -> 87         0.26883
      84 -> 88         0.60074

Excited State  11:   Singlet-B2U     2.6736 eV    f=0.0000
      82 -> 86         0.50887
      83 -> 87        -0.49086

Excited State  25:   Singlet-B2U     3.6158 eV    f=0.0000
      80 -> 88         0.60343
      82 -> 86        -0.15076
      83 -> 87        -0.15364
      84 -> 88         0.13631

Excited State  30:   Singlet-B3U     3.9692 eV    f=0.0188
      75 -> 85        -0.36594
      83 -> 94        -0.10637
      84 -> 90         0.57800

Excited State  35:   Singlet-B2U     4.0857 eV    f=0.0089
      77 -> 87        -0.10377
      78 -> 88         0.61290
      81 -> 89         0.30140

Excited State  38:   Singlet-B1U     4.2204 eV    f=0.0023
      82 -> 90         0.70437

 Excited State  39:   Singlet-B2U    4.2777 eV    f=0.0056
      76 -> 86         0.17646
      77 -> 87         0.24290
      78 -> 88        -0.19631
      81 -> 89         0.58444

 Excited State  40:   Singlet-B1U    4.3265 eV    f=0.0001
      83 -> 91         0.70656

Excited State  45:   Singlet-B3U     4.4240 eV    f=0.0000
      83 -> 92         0.70689
```

```
Excited State  47:   Singlet-B3U     4.4517 eV    f=0.0707
      74 -> 86        -0.16699
      75 -> 85         0.35448
      80 -> 90         0.31832
      83 -> 94        -0.22885
      84 -> 90         0.18687
      84 -> 95         0.34213

 Excited State  48:   Singlet-B2U    4.4796 eV    f=0.0002
      76 -> 86        -0.49269
      77 -> 87         0.49941

Excited State  50:   Singlet-B3U     4.4901 eV    f=0.0057
      75 -> 85        -0.15376
      80 -> 90        -0.20322
      83 -> 94         0.15662
      84 -> 95         0.61592

 Excited State  51:   Singlet-B2U    4.4902 eV     f=0.0000
      79 -> 89         0.70205

Excited State  53:   Singlet-B1U     4.4994 eV     f=0.0016
      73 -> 85         0.68753
      75 -> 87        -0.11425

 Excited State  54:   Singlet-B3U    4.5364 eV     f=0.0005
      81 -> 91         0.70167

Excited State  56:   Singlet-B1U     4.5768 eV     f=0.0001
      84 -> 96         0.70685

Excited State  59:   Singlet-B1U     4.6321 eV     f=0.0009
      81 -> 92         0.70726

Excited State  63:   Singlet-B3U     4.7084 eV     f=0.0410
      75 -> 85        -0.24352
      78 -> 90        -0.10466
      79 -> 91         0.12209
      80 -> 90         0.54222
      83 -> 94         0.29078

 Excited State  64:   Singlet-B1U    4.7112 eV     f=0.0000
      75 -> 87         0.67829
      79 -> 94        -0.11025

Excited State  66:   Singlet-B2U     4.7524 eV     f=0.0247
      71 -> 85         0.24094
      76 -> 86         0.34822
      77 -> 87         0.28837
      82 -> 93         0.41464
      83 -> 98         0.19009

 Excited State  67:   Singlet-B1U    4.7657 eV     f=0.0001
      84 -> 99         0.70222

Excited State  72:   Singlet-B3U     4.8447 eV     f=0.0029
      79 -> 91         0.66103
      83 -> 94        -0.21862

 Excited State  73:   Singlet-B2U    4.8692 eV     f=0.0047
      71 -> 85        -0.29901
      82 -> 93         0.49679
      83 -> 98        -0.37959

Excited State  75:   Singlet-B3U     4.8896 eV     f=0.0153
      74 -> 86         0.39745
      75 -> 85        -0.13123
      79 -> 91        -0.19317
      80 -> 90         0.17085
      82 -> 96        -0.17783
      82 -> 99         0.17871
      83 -> 94        -0.37913
      84 ->101         0.10777

 Excited State  76:   Singlet-B1U    4.9014 eV     f=0.0003
      82 -> 95         0.70646

Excited State  80:   Singlet-B2U     4.9362 eV     f=0.0001
      71 -> 85        -0.14687
      83 -> 98         0.15522
      84 ->100         0.67352

 Excited State  81:   Singlet-B1U    4.9400 eV     f=0.0029
      79 -> 92         0.70399

Excited State  83:   Singlet-B1U     4.9493 eV     f=0.0079
      81 -> 94         0.69355

 Excited State  84:   Singlet-B2U    4.9510 eV     f=0.0010
      71 -> 85         0.46986
      83 -> 98        -0.46745
      84 ->100         0.21424

Excited State  86:   Singlet-B3U     4.9726 eV     f=0.0049
      73 -> 87        -0.35338
      74 -> 86         0.39902
      82 -> 96         0.39598
      82 -> 99        -0.11959
      83 -> 94         0.13475

Excited State  89:   Singlet-B3U     5.0257 eV     f=0.0062
      73 -> 87         0.24042
      74 -> 86        -0.11929
      82 -> 96         0.53793
      82 -> 99         0.25957
      83 -> 94        -0.16115
      84 ->101         0.17157

Excited State  93:   Singlet-B3U     5.1196 eV     f=0.0012
      78 -> 90         0.15648
      82 -> 99        -0.21808
      84 ->101         0.64684

 Excited State  94:   Singlet-B2U    5.1344 eV      f=0.0025
      81 -> 97         0.70304
```

---

4. bisfulvalenide radical cation (Fc=Fc.+)

a. calculated by ADF

```
    1.XX       -2.162155   -2.015309    0.000000
    2.C        -1.792764   -0.731363    0.000000
    3.C        -1.725136   -1.582680   -1.161463
    4.C        -1.660379   -2.940811   -0.715803
    5.C        -1.660379   -2.940811    0.715803
    6.C        -1.725136   -1.582680    1.161463
    7.H        -1.745816   -1.256620   -2.197107
    8.H        -1.613548   -3.817113   -1.355514
    9.H        -1.613548   -3.817113    1.355514
   10.H        -1.745816   -1.256620    2.197107
   11.Fe        0.000000   -1.888849    0.000000
   12.XX        2.162155   -2.015309    0.000000
   13.C         1.792764   -0.731363    0.000000
   14.C         1.725136   -1.582680    1.161463
   15.C         1.725136   -1.582680   -1.161463
   16.C         1.660379   -2.940811    0.715803
   17.H         1.745816   -1.256620    2.197107
   18.C         1.660379   -2.940811   -0.715803
   19.H         1.745816   -1.256620   -2.197107
   20.H         1.613548   -3.817113    1.355514
   21.H         1.613548   -3.817113   -1.355514
   22.C        -1.792764    0.731363    0.000000
   23.XX       -2.162155    2.015309    0.000000
   24.C        -1.725136    1.582680    1.161463
   25.C        -1.725136    1.582680   -1.161463
   26.C        -1.660379    2.940811    0.715803
   27.H        -1.745816    1.256620    2.197107
   28.C        -1.660379    2.940811   -0.715803
   29.H        -1.745816    1.256620   -2.197107
   30.H        -1.613548    3.817113    1.355514
   31.H        -1.613548    3.817113   -1.355514
   32.Fe        0.000000    1.888849    0.000000
   33.XX        2.162155    2.015309    0.000000
   34.C         1.792764    0.731363    0.000000
   35.C         1.725136    1.582680   -1.161463
   36.C         1.725136    1.582680    1.161463
   37.C         1.660379    2.940811   -0.715803
   38.H         1.745816    1.256620   -2.197107
   39.C         1.660379    2.940811    0.715803
   40.H         1.745816    1.256620    2.197107
   41.H         1.613548    3.817113   -1.355514
   42.H         1.613548    3.817113    1.355514
```

Symmetry B1.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x)	mu (y)	mu (z)
1	0.75861	0.50927E-04	0.0000	0.0000	-0.52346E-01
2	2.3249	0.35487E-03	0.0000	0.0000	-0.78932E-01
3	4.1093	0.10234E-03	0.0000	0.0000	-0.31882E-01
4	4.3276	0.10422E-02	0.0000	0.0000	-0.99145E-01
6	4.5344	0.23996E-02	0.0000	0.0000	-0.14697
9	4.8499	0.23434E-02	0.0000	0.0000	0.14044
10	4.9384	0.27815E-03	0.0000	0.0000	-0.47948E-01
12	5.1885	0.73841E-03	0.0000	0.0000	-0.76216E-01
13	5.2059	0.20222E-03	0.0000	0.0000	0.39818E-01
14	5.2722	0.55120E-03	0.0000	0.0000	-0.65325E-01

Major MO -> MO transitions for the above excitations

Excit. No.	Occ.	to	virt.	Contrib. (sum=1)	transition moment x	y	z
1: Beta	6b3.g	->	9b2.u	0.9994	0.0000	0.0000	-0.1830
2: Beta	5b3.g	->	9b2.u	0.9997	0.0000	0.0000	-0.2130

```
3: Alph 5b2.g  ->  9b3.u   0.7507  0.0000  0.0000 -0.2871
3: Beta 5b2.g  ->  9b3.u   0.2057  0.0000  0.0000  0.1621

4: Beta 5b2.g  ->  9b3.u   0.7183  0.0000  0.0000 -0.2952
4: Alph 5b2.g  ->  9b3.u   0.2184  0.0000  0.0000 -0.1509

6: Beta 6b1.u  ->  11a.g   0.5716  0.0000  0.0000 -0.3330
6: Alph 6b1.u  ->  11a.g   0.4156  0.0000  0.0000 -0.2830

10: Beta 4b3.g  ->  9b2.u  0.9941  0.0000  0.0000 -0.1688

12: Beta 9a.g   ->  7b1.u  0.7639  0.0000  0.0000 -0.1341
12: Beta 5a.u   ->  8b1.g  0.0906  0.0000  0.0000 -0.0696
12: Alph 10a.g  ->  7b1.u  0.0541  0.0000  0.0000 -0.0720

13: Alph 8b3.u  ->  6b2.g  0.5556  0.0000  0.0000  0.2185
13: Alph 5a.u   ->  8b1.g  0.2092  0.0000  0.0000  0.0964
13: Beta 5a.u   ->  8b1.g  0.1370  0.0000  0.0000  0.0855
13: Beta 9a.g   ->  7b1.u  0.0606  0.0000  0.0000 -0.0377

14: Alph 10a.g  ->  7b1.u  0.2929  0.0000  0.0000 -0.1661
14: Beta 5a.u   ->  8b1.g  0.1981  0.0000  0.0000  0.1022
14: Alph 8b3.u  ->  6b2.g  0.1509  0.0000  0.0000 -0.1131
14: Beta 8b2.u  ->  7b3.g  0.1205  0.0000  0.0000  0.1567
14: Beta 8b3.u  ->  6b2.g  0.0896  0.0000  0.0000  0.0764
14: Alph 9b2.u  ->  7b3.g  0.0823  0.0000  0.0000 -0.2127
```

Symmetry B2.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	0.94664	0.72688E-02	0.0000	0.55984	0.0000
2	1.2854	0.24163E-01	0.0000	0.87593	0.0000
3	3.4509	0.38690E-02	0.0000	0.21392	0.0000
4	3.4808	0.28904E-01	0.0000	-0.58219	0.0000
5	4.1020	0.38647E-02	0.0000	0.19610	0.0000
6	4.2579	0.57550E-03	0.0000	-0.74275E-01	0.0000
8	4.5265	0.25762E-02	0.0000	-0.15241	0.0000
9	4.6175	0.18780	0.0000	1.2884	0.0000
10	4.8552	0.70143E-02	0.0000	-0.24283	0.0000
11	4.8869	0.35348E-03	0.0000	0.54336E-01	0.0000
12	5.0309	0.20539E-02	0.0000	-0.12909	0.0000
13	5.1578	0.28887E-02	0.0000	-0.15120	0.0000
14	5.2125	0.21321E-01	0.0000	-0.40860	0.0000
15	5.3531	0.64274E-01	0.0000	-0.70006	0.0000
16	5.4481	0.30224E-02	0.0000	0.15048	0.0000

Major MO -> MO transitions for the above excitations

Excit. No.	Occ.	to	virt.	Contrib. sum=1)	transition moment x	y	z
1: Beta 10a.g	->		9b2.u	0.7613	0.0000	1.7267	0.0000
1: Beta 9a.g	->		9b2.u	0.2299	0.0000	-0.6804	0.0000
2: Beta 9a.g	->		9b2.u	0.7503	0.0000	1.0549	0.0000
2: Beta 10a.g	->		9b2.u	0.2100	0.0000	0.7782	0.0000
3: Beta 7b1.g	->		9b3.u	0.4864	0.0000	-0.8101	0.0000
3: Alph 7b1.g	->		9b3.u	0.4259	0.0000	0.7436	0.0000
4: Beta 8a.g	->		9b2.u	0.9492	0.0000	-1.2115	0.0000
5: Alph 9b2.u	->		11a.g	0.6676	0.0000	1.3259	0.0000
5: Alph 7b1.g	->		9b3.u	0.1914	0.0000	-0.4572	0.0000
5: Beta 7b1.g	->		9b3.u	0.1005	0.0000	-0.3378	0.0000
6: Beta 8b2.u	->		11a.g	0.4675	0.0000	0.0939	0.0000
6: Alph 8b2.u	->		11a.g	0.2275	0.0000	0.0713	0.0000
6: Alph 5a.u	->		6b2.g	0.0918	0.0000	0.0001	0.0000
6: Beta 5a.u	->		6b2.g	0.0509	0.0000	-0.0023	0.0000
7: Alph 5a.u	->		6b2.g	0.2621	0.0000	-0.0002	0.0000
7: Beta 8b2.u	->		11a.g	0.2310	0.0000	0.0647	0.0000
7: Beta 5a.u	->		6b2.g	0.2244	0.0000	0.0048	0.0000
7: Beta 5b2.g	->		6a.u	0.0857	0.0000	-0.0296	0.0000
7: Alph 5b2.g	->		6a.u	0.0728	0.0000	0.0277	0.0000
8: Alph 8b2.u	->		11a.g	0.6785	0.0000	-0.1195	0.0000
8: Beta 8b2.u	->		11a.g	0.2361	0.0000	0.0647	0.0000
9: Beta 7b1.g	->		9b3.u	0.2889	0.0000	0.5397	0.0000
9: Alph 7b1.g	->		9b3.u	0.2100	0.0000	0.4514	0.0000
9: Alph 9b2.u	->		11a.g	0.2063	0.0000	0.6947	0.0000
9: Beta 6b3.g	->		7b1.u	0.0800	0.0000	0.0479	0.0000
10: Beta 6b3.g	->		7b1.u	0.3072	0.0000	0.0915	0.0000
10: Alph 6b3.g	->		7b1.u	0.2502	0.0000	-0.0646	0.0000
10: Alph 5a.u	->		6b2.g	0.1913	0.0000	-0.0002	0.0000
10: Alph 5b2.g	->		6a.u	0.1258	0.0000	-0.0348	0.0000
11: Alph 5b2.g	->		6a.u	0.3716	0.0000	0.0596	0.0000
11: Alph 5a.u	->		6b2.g	0.2194	0.0000	0.0002	0.0000
11: Beta 6b3.g	->		7b1.u	0.2015	0.0000	0.0739	0.0000
11: Beta 5a.u	->		6b2.g	0.1614	0.0000	0.0039	0.0000
12: Beta 5b2.g	->		6a.u	0.4963	0.0000	-0.0668	0.0000
12: Beta 5a.u	->		6b2.g	0.3397	0.0000	-0.0055	0.0000
12: Alph 5b2.g	->		6a.u	0.0829	0.0000	0.0278	0.0000
12: Alph 6b3.g	->		7b1.u	0.0610	0.0000	-0.0313	0.0000
13: Alph 7b2.u	->		11a.g	0.4837	0.0000	0.7420	0.0000
13: Beta 7b2.u	->		11a.g	0.4552	0.0000	-0.8727	0.0000
15: Beta 7b2.u	->		11a.g	0.4421	0.0000	-0.8442	0.0000
15: Alph 7b2.u	->		11a.g	0.4133	0.0000	-0.6733	0.0000
15: Beta 6b1.u	->		7b3.g	0.0633	0.0000	0.1380	0.0000
16: Beta 6b1.u	->		7b3.g	0.4334	0.0000	0.3580	0.0000
16: Alph 6b1.u	->		7b3.g	0.1994	0.0000	-0.2347	0.0000
16: Alph 6b3.g	->		7b1.u	0.0917	0.0000	0.0369	0.0000
16: Alph 8b3.u	->		8b1.g	0.0901	0.0000	-0.2770	0.0000
16: Beta 8b3.u	->		8b1.g	0.0503	0.0000	0.2045	0.0000

Symmetry B3.u

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	1.8002	0.75213E-05	-0.13059E-01	0.0000	0.0000
2	2.0603	0.69777E-05	-0.11757E-01	0.0000	0.0000
3	2.3021	0.38810E-03	-0.82952E-01	0.0000	0.0000
5	2.5969	0.91206E-03	-0.11973	0.0000	0.0000
6	2.7542	0.15572E-02	-0.15191	0.0000	0.0000
7	2.8175	0.74548E-05	-0.10392E-01	0.0000	0.0000
8	2.8857	0.15192E-02	0.14659	0.0000	0.0000
9	2.8977	0.41150E-02	-0.24076	0.0000	0.0000
10	3.0035	0.11903E-02	0.12719	0.0000	0.0000
11	3.1435	0.15957E-02	0.14394	0.0000	0.0000
12	3.6203	0.17113E-03	-0.43925E-01	0.0000	0.0000
13	3.8512	0.18811E-03	0.44650E-01	0.0000	0.0000
14	4.0356	0.42283E-03	0.65395E-01	0.0000	0.0000
15	4.0708	0.47225E-02	0.21761	0.0000	0.0000
17	4.2217	0.60419E-02	-0.24169	0.0000	0.0000
18	4.3928	0.25020E-04	-0.15247E-01	0.0000	0.0000
19	4.4191	0.49446E-03	-0.67581E-01	0.0000	0.0000
20	4.4867	0.17842E-03	-0.40289E-01	0.0000	0.0000
21	4.5850	0.11557E-01	-0.32076	0.0000	0.0000
23	4.9131	0.39902E-02	-0.18207	0.0000	0.0000
24	5.0402	0.89867E-01	-0.85309	0.0000	0.0000
25	5.2049	0.17238E-01	-0.36767	0.0000	0.0000

Major MO -> MO transitions for the above excitations

Excit.	Occ.	to	virt.	Contrib.	transition moment		
1: Beta 10a.g	->		9b3.u	0.7744	0.2012	0.0000	0.0000
1: Alph 10a.g	->		9b3.u	0.1931	-0.0393	0.0000	0.0000
2: Beta 9a.g	->		9b3.u	0.5273	0.0278	0.0000	0.0000
2: Alph 10a.g	->		9b3.u	0.3023	0.0460	0.0000	0.0000
2: Beta 10a.g	->		9b3.u	0.0917	0.0647	0.0000	0.0000
3: Alph 10a.g	->		9b3.u	0.4475	-0.0529	0.0000	0.0000
3: Beta 9a.g	->		9b3.u	0.3845	0.0224	0.0000	0.0000
3: Beta 10a.g	->		9b3.u	0.0881	-0.0600	0.0000	0.0000
5: Alph 9a.g	->		9b3.u	0.5080	0.0039	0.0000	0.0000
5: Beta 7b1.g	->		9b2.u	0.4012	-0.6155	0.0000	0.0000
5: Beta 9a.g	->		9b3.u	0.0628	-0.0085	0.0000	0.0000
6: Beta 7b1.g	->		9b2.u	0.5213	-0.6814	0.0000	0.0000
6: Alph 9a.g	->		9b3.u	0.4109	-0.0034	0.0000	0.0000
7: Alph 6b1.u	->		6b2.g	0.5198	0.0055	0.0000	0.0000
7: Alph 6b3.g	->		6a.u	0.4741	-0.1281	0.0000	0.0000
8: Beta 6b3.g	->		6a.u	0.4113	-0.0930	0.0000	0.0000
8: Alph 9b2.u	->		8b1.g	0.2885	0.7583	0.0000	0.0000
8: Beta 6b1.u	->		6b2.g	0.2660	0.0082	0.0000	0.0000
9: Alph 9b2.u	->		8b1.g	0.5939	-1.0857	0.0000	0.0000
9: Beta 6b1.u	->		6b2.g	0.2654	0.0081	0.0000	0.0000
9: Beta 6b3.g	->		6a.u	0.0868	-0.0426	0.0000	0.0000
10: Beta 8b2.u	->		8b1.g	0.6855	0.4837	0.0000	0.0000
10: Alph 8b2.u	->		8b1.g	0.2431	-0.1584	0.0000	0.0000
11: Alph 8b2.u	->		8b1.g	0.4179	0.2030	0.0000	0.0000
11: Beta 6b1.u	->		6b2.g	0.1360	0.0056	0.0000	0.0000
11: Beta 6b3.g	->		6a.u	0.1128	0.0466	0.0000	0.0000
11: Alph 6b1.u	->		6b2.g	0.1087	0.0024	0.0000	0.0000
11: Alph 6b3.g	->		6a.u	0.0953	0.0544	0.0000	0.0000
11: Beta 8b2.u	->		8b1.g	0.0894	0.1708	0.0000	0.0000
12: Alph 8b2.u	->		8b1.g	0.2912	0.1579	0.0000	0.0000

```
12: Beta 8b2.u  ->  8b1.g   0.1579  0.2115  0.0000  0.0000
12: Beta 6b1.u  ->  6b2.g   0.1122 -0.0047  0.0000  0.0000
12: Beta 6b3.g  ->  6a.u    0.1065 -0.0422  0.0000  0.0000
12: Alph 6b1.u  ->  6b2.g   0.0985 -0.0021  0.0000  0.0000
12: Alph 6b3.g  ->  6a.u    0.0934 -0.0501  0.0000  0.0000

13: Beta 7b2.u  ->  8b1.g   0.5613  1.4769  0.0000  0.0000
13: Alph 7b2.u  ->  8b1.g   0.3391 -1.0079  0.0000  0.0000

14: Alph 7b2.u  ->  8b1.g   0.4491  1.1331  0.0000  0.0000
14: Alph 5b3.g  ->  6a.u    0.3545 -1.1925  0.0000  0.0000
14: Beta 7b2.u  ->  8b1.g   0.0969  0.5995  0.0000  0.0000
14: Alph 5b1.u  ->  6b2.g   0.0697 -0.5329  0.0000  0.0000

15: Beta 10a.g  ->  10b3.u  0.4206 -0.9051  0.0000  0.0000
15: Beta 7b2.u  ->  8b1.g   0.2109  0.8806  0.0000  0.0000
15: Alph 5b3.g  ->  6a.u    0.1781  0.8415  0.0000  0.0000
15: Alph 7b2.u  ->  8b1.g   0.0621  0.4196  0.0000  0.0000
15: Beta 5b3.g  ->  6a.u    0.0555 -0.4610  0.0000  0.0000

17: Beta 10a.g  ->  10b3.u  0.4507 -0.9199  0.0000  0.0000
17: Beta 5b3.g  ->  6a.u    0.2078  0.8762  0.0000  0.0000
17: Beta 5b1.u  ->  6b2.g   0.0969  0.6018  0.0000  0.0000
17: Alph 5b1.u  ->  6b2.g   0.0593 -0.4805  0.0000  0.0000
17: Alph 7b2.u  ->  8b1.g   0.0462 -0.3555  0.0000  0.0000

18: Alph 8a.g   ->  9b3.u   0.6658  1.4074  0.0000  0.0000
18: Beta 5b3.g  ->  6a.u    0.1771 -0.7930  0.0000  0.0000
18: Beta 8a.g   ->  9b3.u   0.1212 -0.5884  0.0000  0.0000

19: Beta 5b1.u  ->  6b2.g   0.5277  1.3727  0.0000  0.0000
19: Beta 5b3.g  ->  6a.u    0.3291 -1.0779  0.0000  0.0000
19: Alph 8a.g   ->  9b3.u   0.0854 -0.5027  0.0000  0.0000

20: Beta 9a.g   ->  10b3.u  0.9714  0.3707  0.0000  0.0000

21: Beta 8a.g   ->  9b3.u   0.4473  1.1066  0.0000  0.0000
21: Alph 10a.g  ->  10b3.u  0.1913  0.3158  0.0000  0.0000
21: Beta 5b1.u  ->  6b2.g   0.1549 -0.7303  0.0000  0.0000
21: Beta 5b3.g  ->  6a.u    0.0784 -0.5165  0.0000  0.0000

23: Beta 6b1.g  ->  9b2.u   0.9744  0.0505  0.0000  0.0000

24: Alph 9a.g   ->  10b3.u  0.3845  0.5948  0.0000  0.0000
24: Beta 6b1.u  ->  7b2.g   0.1145  0.4072  0.0000  0.0000
24: Beta 8a.g   ->  9b3.u   0.0959 -0.4887  0.0000  0.0000
24: Alph 8a.g   ->  9b3.u   0.0564 -0.3825  0.0000  0.0000
24: Beta 6b3.g  ->  7a.u    0.0502  0.2531  0.0000  0.0000
24: Beta 5b1.u  ->  6b2.g   0.0481 -0.3881  0.0000  0.0000

25: Alph 9a.g   ->  10b3.u  0.4842 -0.6568  0.0000  0.0000
25: Beta 6b1.u  ->  7b2.g   0.3836  0.7334  0.0000  0.0000
25: Beta 6b3.g  ->  7a.u    0.0661  0.2857  0.0000  0.0000
```

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b) Fc=Fc.+ calculated by Gaussian 03

```
  6          0.733308    1.811327    0.000000
  6          1.591841    1.727398    1.177652
  6          2.969110    1.655694    0.726255
  6          2.969110    1.655694   -0.726255
  6          1.591841    1.727398   -1.177652
  1          1.266667    1.771589    2.216294
  1          3.848545    1.616538    1.368083
  1          3.848545    1.616538   -1.368083
  1          1.266667    1.771589   -2.216294
 26          1.891535    0.000000    0.000000
  6          0.733308   -1.811327    0.000000
  6          1.591841   -1.727398   -1.177652
  6          1.591841   -1.727398    1.177652
  6          2.969110   -1.655694   -0.726255
  1          1.266667   -1.771589   -2.216294
  6          2.969110   -1.655694    0.726255
  1          1.266667   -1.771589    2.216294
  1          3.848545   -1.616538   -1.368083
  1          3.848545   -1.616538    1.368083
  6         -0.733308    1.811327    0.000000
  6         -1.591841    1.727398   -1.177652
  6         -1.591841    1.727398    1.177652
  6         -2.969110    1.655694   -0.726255
  1         -1.266667    1.771589   -2.216294
  6         -2.969110    1.655694    0.726255
  1         -1.266667    1.771589    2.216294
  1         -3.848545    1.616538   -1.368083
  1         -3.848545    1.616538    1.368083
 26         -1.891535    0.000000    0.000000
  6         -0.733308   -1.811327    0.000000
  6         -1.591841   -1.727398    1.177652
  6         -1.591841   -1.727398   -1.177652
  6         -2.969110   -1.655694    0.726255
  1         -1.266667   -1.771589    2.216294
  6         -2.969110   -1.655694   -0.726255
  1         -1.266667   -1.771589   -2.216294
  1         -3.848545   -1.616538    1.368083
  1         -3.848545   -1.616538   -1.368083
```

```
Sum of electronic and zero-point Energies=   -1018.247926
Sum of electronic and thermal Energies=      -1018.230784
Sum of electronic and thermal Enthalpies=    -1018.229840
Sum of electronic and thermal Free Energies= -1018.289673

Molecular orbitals involved in electronic excitations:

MO  symmetry
71   8ag
73   5b2g
74   5au
75   7b1g
76   5b1u
77   5b3g
78   7b2u
79   9ag
80   8b2u
81   10ag
82   6b1u
83   6b3g
84   9b2u
85   9b3u
86   6b2g
87   6au
88   8b1g
89   10b3u
90   11ag
91   10b2u
92   7b1u
93   7b2g
94   8b1u
95   12ag
96   7b3g
97   11b3u
98   7au
99   8b3g
100  9b1g
101  13ag

Excitation energies and oscillator strengths:

 Excited State   1:   ?Spin  -B1U     0.6710 eV  f=0.0001
      82B -> 84B        1.21259

Excited State   3:   ?Spin  -B3U     0.8834 eV  f=0.0206
      75A -> 85A        0.19823
      81A -> 89A        0.11791
      84A -> 89A       -0.16683
      79B -> 84B        0.24923
      83B -> 84B        0.86654


 Excited State   5:   ?Spin  -B3U     1.2067 eV  f=0.0103
      75A -> 85A       -0.17796
      84A -> 89A        0.10454
      75B -> 85B       -0.15105
      79B -> 84B        0.98712
      83B -> 84B       -0.14381

 Excited State   6:   ?Spin  -B2U     1.4755 eV f=0.0003
      79A -> 85A        0.22226
      80A -> 85A       -0.37917
      81A -> 88A       -0.16529
      84A -> 88A        0.14049
      75B -> 84B       -0.25425
      80B -> 86B        0.14814
      82B -> 87B        0.15313
      83B -> 85B        0.98320

Excited State  12:   ?Spin  -B2U     1.7618 eV  f=0.0002
      78A -> 88A       -0.13329
      79A -> 85A       -0.34460
      80A -> 85A       -0.59970
      81A -> 88A       -0.19477
      82A -> 86A       -0.10504
      83A -> 87A       -0.10897
      84A -> 88A       -0.14641
      75B -> 84B        0.16261
      78B -> 88B        0.11737
      79B -> 85B        0.82036
      81B -> 88B        0.28610

Excited State  17:   ?Spin  -B2U     2.1661 eV  f=0.0003
      79A -> 85A       -0.16044
      80A -> 85A        0.11178
      82A -> 86A        0.57347
      83A -> 87A        0.61784
      75B -> 84B        0.17085
      79B -> 85B        0.21074
      80B -> 86B       -0.42449
      82B -> 87B       -0.45049
      83B -> 85B        0.25686

Excited State  20:   ?Spin  -B2U     2.2896 eV  f=0.0005
      79A -> 85A       -0.11500
      80A -> 85A        0.70175
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     83A -> 87A       -0.10076
     75B -> 84B        0.29635
     79B -> 85B        0.41857
     80B -> 86B        0.30325
     82B -> 87B        0.32565
     83B -> 85B        0.24226

 Excited State  21:   ?Spin  -B1U    2.2899 eV  f=0.0004
     77B -> 84B        1.00062

Excited State  25:   ?Spin  -B2U     2.4986 eV  f=0.0015
     78A -> 88A       -0.11556
     79A -> 85A       -0.60618
     80A -> 85A       -0.13511
     82A -> 86A       -0.10685
     83A -> 87A       -0.10882
     84A -> 88A       -0.14796
     75B -> 84B        0.59202
     79B -> 85B       -0.46499
     83B -> 85B        0.14061

Excited State  27:   ?Spin  -B2U     2.6230 eV  f=0.0001
     79A -> 85A        0.61140
     80A -> 85A       -0.11738
     82A -> 86A       -0.11322
     83A -> 87A       -0.12626
     84A -> 88A        0.31099
     75B -> 84B        0.66857
     80B -> 86B       -0.16309
     82B -> 87B       -0.18044

Excited State  32:   ?Spin  -B2U     2.8517 eV   f=0.0001
     79A -> 85A        0.10294
     82A -> 86A       -0.68483
     83A -> 87A        0.68590
     84A -> 88A       -0.20612

Excited State  34:   ?Spin  -B2U     2.8667 eV   f=0.0067
     79A -> 85A       -0.36865
     82A -> 86A       -0.22075
     83A -> 87A        0.12155
     84A -> 88A        0.84506
     75B -> 84B       -0.10102
     81B -> 88B       -0.18754
     82B -> 87B       -0.11027

Excited State  40:   ?Spin  -B3U     2.9911 eV   f=0.0017
     71A -> 88A       -0.16296
     74A -> 86A       -0.10899
     75A -> 85A       -0.73152
     71B -> 88B        0.16517
     73B -> 87B        0.10244
     74B -> 86B        0.11419
     75B -> 85B        0.76771
Excited State  42:   ?Spin  -B2U     3.0222 eV   f=0.0004
     80B -> 86B       -0.66993
     81B -> 88B        0.11625
     82B -> 87B        0.72294

Excited State  44:   ?Spin  -B2U     3.0303 eV   f=0.0026
     80A -> 85A        0.10181
     81A -> 88A       -0.32890
     82A -> 86A        0.12566
     83A -> 87A        0.12601
     84A -> 88A        0.21494
     79B -> 85B       -0.15973
     80B -> 86B        0.18887
     81B -> 88B        0.86210

Excited State  48:   ?Spin  -B2U     3.1126 eV   f=0.0010
     80A -> 85A       -0.17150
     81A -> 88A        0.72427
     82A -> 86A        0.28877
     83A -> 87A        0.25654
     84A -> 88A        0.13637
     80B -> 86B        0.41441
     82B -> 87B        0.30030

Excited State  58:   ?Spin  -B3U     3.4082 eV   f=0.0316
     75A -> 85A        0.14927
     72B -> 84B        0.97454

Excited State  64:   ?Spin  -B2U     3.6230 eV   f=0.0000
     78A -> 88A        0.19425
     80A -> 85A        0.10843
     81A -> 88A        0.55878
     82A -> 86A       -0.25461
     83A -> 87A       -0.24129
     75B -> 84B       -0.12059
     78B -> 88B       -0.11028
     80B -> 86B       -0.28149
     81B -> 88B        0.38846
     82B -> 87B       -0.26784
     83B -> 89B        0.11182

Excited State  68:   ?Spin  -B2U     3.7387 eV   f=0.0000
     72A -> 85A       -0.10992
     76A -> 86A        0.25490
     77A -> 87A        0.31517
     78A -> 88A       -0.45437
     81A -> 88A        0.11343
     76B -> 86B       -0.11452
     77B -> 87B       -0.13793
     78B -> 88B        0.73538
     83B -> 89B        0.19632

 Excited State  69:   ?Spin  -B1U    3.7691 eV   f=0.0000
     71A -> 86A        0.12165
     73A -> 85A        0.75729
     74A -> 88A        0.15138
     75A -> 87A        0.28041
     71B -> 86B       -0.11946
     73B -> 85B       -0.54091
     74B -> 88B       -0.15718
     75B -> 87B       -0.26969

Excited State  72:   ?Spin  -B2U     3.9102 eV   f=0.0025
     76A -> 86A        0.30876
     77A -> 87A        0.68632
     78A -> 88A        0.48579
     76B -> 86B       -0.23639
     77B -> 87B       -0.26668
     78B -> 88B       -0.19148
     83B -> 89B        0.20775

Excited State  74:   ?Spin  -B3U     3.9262 eV   f=0.0002
     73A -> 87A        0.46888
     74A -> 86A        0.62449
     75A -> 85A       -0.25760
     73B -> 87B       -0.40610
     74B -> 86B       -0.51416
     81B -> 90B       -0.12468
     82B -> 91B       -0.10124

Excited State  76:   ?Spin  -B2U     3.9977 eV   f=0.0050
     72A -> 85A       -0.20307
     76A -> 86A       -0.11216
     78A -> 88A        0.61564
     76B -> 86B        0.17203
     77B -> 87B        0.21328
     78B -> 88B        0.54258
     83B -> 89B       -0.42943

 Excited State  77:   ?Spin  -B3U     4.0080 eV   f=0.0000
     75A -> 85A        0.41035
     84A -> 89A        0.75989
     73B -> 87B       -0.14412
     74B -> 86B       -0.18794
     75B -> 85B        0.41475

 Excited State  78:   ?Spin  -B2U    4.0118 eV    f=0.0000
     76A -> 86A        0.81909
     77A -> 87A       -0.53105
     78A -> 88A        0.17780

Excited State  82:   ?Spin  -B1U     4.1207 eV    f=0.0015
     73A -> 85A        0.62008
     75A -> 87A       -0.20344
     73B -> 85B        0.73927

Excited State  84:   ?Spin  -B2U     4.1492 eV    f=0.0013
     72A -> 85A       -0.41839
     76A -> 86A       -0.10263
     78A -> 88A        0.18340
     76B -> 86B        0.21283
     77B -> 87B        0.32766
     83B -> 89B        0.77391

Excited State  87:   ?Spin  -B2U     4.2183 eV   f=0.0010
     72A -> 85A        0.76036
     72B -> 85B       -0.45745
     76B -> 86B        0.16155
     77B -> 87B        0.32996
     78B -> 88B        0.16195
     83B -> 89B        0.23168

Excited State  91:   ?Spin  -B1U     4.3392 eV   f=0.0000
     71A -> 86A        0.10100
     73A -> 85A       -0.19571
     74A -> 88A        0.16402
     75A -> 87A        0.70202
     71B -> 86B       -0.10584
     73B -> 85B        0.39728
     74B -> 88B       -0.18753
     75B -> 87B       -0.49545

 Excited State  92:   ?Spin  -B2U    4.3425 eV   f=0.0007
     72B -> 85B       -0.14610
     76B -> 86B        0.71175
     77B -> 87B       -0.67502

 Excited State  93:   ?Spin  -B3U    4.3547 eV  f=0.0163
     75A -> 85A        0.14940
     81A -> 89A       -0.44988
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```
     84A -> 89A       -0.28570
     73B -> 87B       -0.13007
     74B -> 86B       -0.20994
     75B -> 85B        0.12960
     81B -> 90B        0.78819

Excited State  96:   ?Spin  -B1U     4.3860 eV   f=0.0000
     82A -> 89A        0.80458
     80B -> 90B       -0.55619
     83B -> 91B       -0.23479

Excited State 100:   ?Spin  -B2U     4.4610 eV   f=0.0042
     72A -> 85A        0.26360
     76A -> 86A        0.17947
     77A -> 87A        0.15186
     72B -> 85B        0.77301
     76B -> 86B        0.42219
     77B -> 87B        0.24666

Excited State 103:   ?Spin  -B3U     4.5080 eV  f=0.1542
     74A -> 86A       -0.25673
     75A -> 85A        0.26854
     81A -> 89A        0.49476
     83A -> 91A       -0.11454
     84A -> 89A       -0.46206
     73B -> 87B       -0.11746
     74B -> 86B       -0.24930
     75B -> 85B        0.36113
     78B -> 90B       -0.12015
     81B -> 90B       -0.16043
     82B -> 91B       -0.18821
```